



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:08 AM UTC

PDB ID : 2AQ3 / pdb_00002aq3
Title : Crystal structure of T-cell receptor V beta domain variant complexed with superantigen SEC3
Authors : Cho, S.; Swaminathan, C.P.; Yang, J.; Kerzic, M.C.; Guan, R.; Kieke, M.C.; Kranz, D.M.; Mariuzza, R.A.; Sundberg, E.J.
Deposited on : 2005-08-17
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

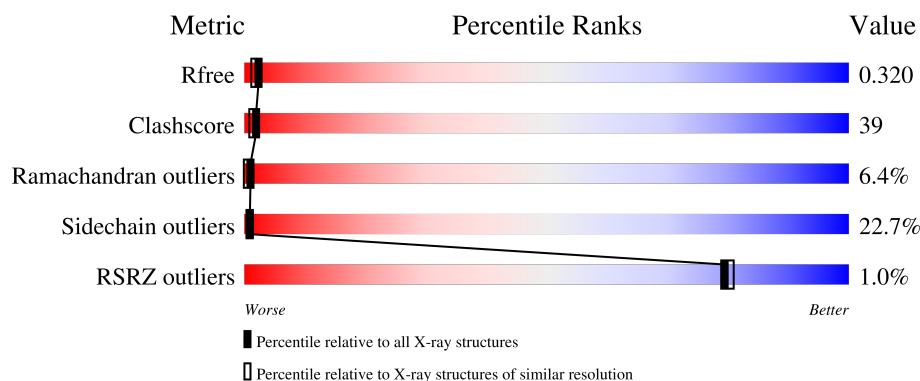
1 Overall quality at a glance

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	112	
1	C	112	
1	E	112	
1	G	112	
2	B	237	

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Mol	Chain	Length	Quality of chain
2	D	237	% 22%43%28%7%
2	F	237	19%47%22%11%
2	H	237	3% 25%39%28%8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11155 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 V.

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	234	Total	C	N	O	S	0	0	0
			1904	1207	312	375	10			
2	D	235	Total	C	N	O	S	0	0	0
			1913	1211	314	378	10			
2	F	234	Total	C	N	O	S	0	0	0
			1906	1205	312	379	10			
2	H	237	Total	C	N	O	S	0	0	0
			1922	1215	315	382	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP P0A0L5
B	?	-	VAL	deletion	UNP P0A0L5
D	?	-	ASN	deletion	UNP P0A0L5
D	?	-	VAL	deletion	UNP P0A0L5
F	?	-	ASN	deletion	UNP P0A0L5
F	?	-	VAL	deletion	UNP P0A0L5
H	?	-	ASN	deletion	UNP P0A0L5
H	?	-	VAL	deletion	UNP P0A0L5

- Molecule 3 is water.

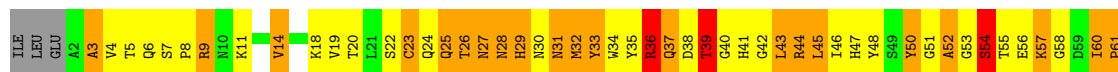
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	48	Total 48	O 48	0	0
3	C	15	Total 15	O 15	0	0
3	D	31	Total 31	O 31	0	0
3	E	11	Total 11	O 11	0	0
3	F	31	Total 31	O 31	0	0
3	G	15	Total 15	O 15	0	0
3	H	26	Total 26	O 26	0	0

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 V

Chain A: 

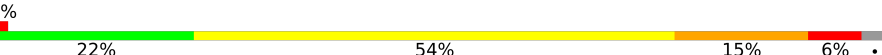


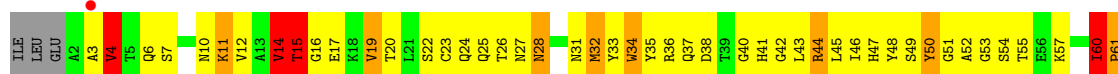
• Molecule 1: T-cell receptor beta chain V

Chain C: 



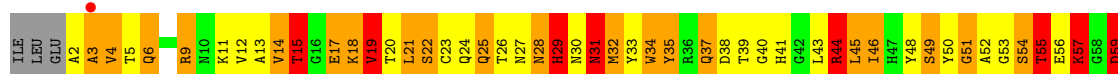
• Molecule 1: T-cell receptor beta chain V

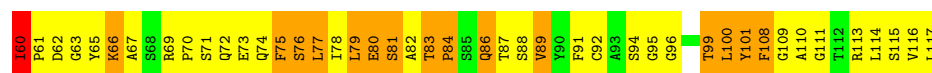
Chain E: 



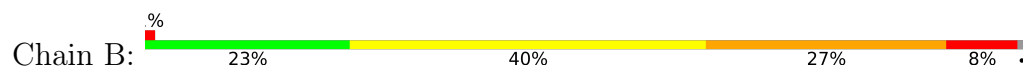
• Molecule 1: T-cell receptor beta chain V

Chain G: 

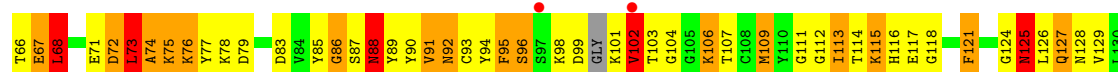
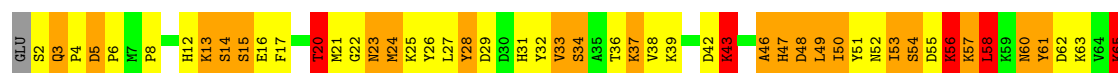
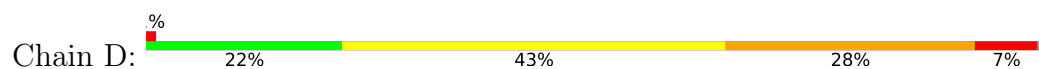




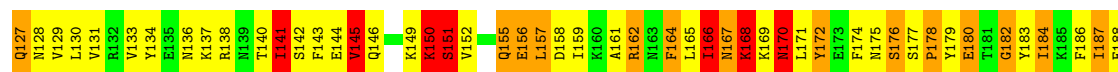
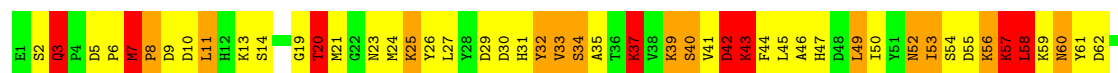
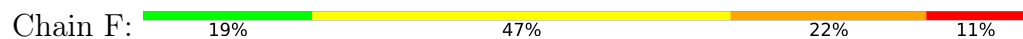
• Molecule 2: Enterotoxin type C-3



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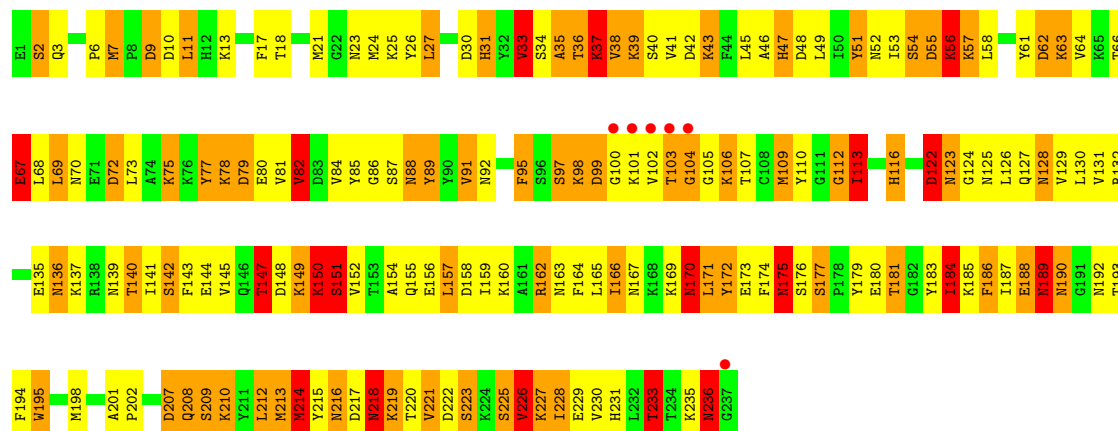
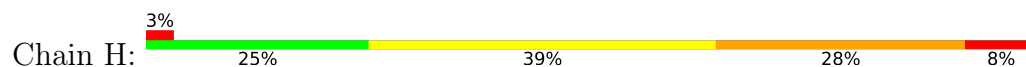


• Molecule 2: Enterotoxin type C-3





• 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	64.16Å 70.46Å 98.37Å 74.18° 75.76° 88.40°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-2.30) 94.2 (40.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.271 0.212 , 0.320	Depositor DCC
R_{free} test set	3402 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11155	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	3.19	70/845 (8.3%)	2.51	59/1142 (5.2%)
1	C	2.84	52/845 (6.2%)	2.41	63/1142 (5.5%)
1	E	2.84	42/846 (5.0%)	2.20	33/1145 (2.9%)
1	G	2.71	51/846 (6.0%)	2.48	49/1145 (4.3%)
2	B	2.46	100/1945 (5.1%)	2.14	78/2619 (3.0%)
2	D	2.20	72/1953 (3.7%)	2.04	76/2627 (2.9%)
2	F	2.20	69/1946 (3.5%)	1.99	63/2618 (2.4%)
2	H	2.13	66/1962 (3.4%)	1.93	56/2640 (2.1%)
All	All	2.47	522/11188 (4.7%)	2.15	477/15078 (3.2%)

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	A	0	6
1	E	0	1
1	G	0	1
2	B	0	5
2	D	0	1
2	F	0	4
2	H	0	1
All	All	0	19

All (522) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	TYR	C-N	38.10	1.87	1.33
1	E	101	TYR	C-N	33.80	1.83	1.33
1	C	63	GLY	C-N	32.44	1.80	1.33
1	E	63	GLY	C-N	29.99	1.76	1.33
1	G	101	TYR	C-N	29.50	1.74	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	65	TYR	C-O	14.98	1.42	1.23
1	A	75	PHE	CA-C	13.54	1.67	1.52
2	B	26	TYR	N-CA	12.95	1.62	1.46
1	A	67	ALA	CA-CB	-11.93	1.32	1.53
1	A	32	MET	SD-CE	11.70	2.08	1.79
1	C	19	VAL	CA-CB	11.52	1.69	1.54
1	G	52	ALA	CA-CB	11.35	1.72	1.53
2	B	27	LEU	N-CA	11.28	1.61	1.46
1	A	60	ILE	CA-CB	11.25	1.68	1.54
1	A	76	SER	N-CA	11.24	1.59	1.46
1	E	51	GLY	N-CA	11.21	1.55	1.45
2	B	166	ILE	CA-C	11.01	1.67	1.52
2	F	203	GLY	C-O	-10.96	1.18	1.24
1	A	52	ALA	CA-CB	10.86	1.70	1.53
1	A	89	VAL	CA-C	10.78	1.65	1.52
1	A	53	GLY	N-CA	-10.56	1.30	1.45
1	C	82	ALA	CA-CB	-10.56	1.35	1.53
1	C	116	VAL	CA-CB	-10.51	1.41	1.53
1	G	45	LEU	C-O	10.50	1.36	1.24
2	B	27	LEU	CG-CD1	10.36	1.86	1.52
1	C	45	LEU	N-CA	10.14	1.58	1.46
1	E	65	TYR	CA-C	10.04	1.65	1.52
2	B	159	ILE	CA-CB	-10.02	1.43	1.54
2	B	164	PHE	C-O	-9.96	1.12	1.24
2	D	145	VAL	CA-CB	9.93	1.66	1.55
2	B	200	PRO	N-CA	-9.77	1.35	1.46
1	C	52	ALA	CA-CB	9.74	1.69	1.53
1	A	44	ARG	CA-C	9.72	1.64	1.52
2	B	24	MET	C-O	9.68	1.36	1.24
1	A	56	GLU	CA-C	9.64	1.64	1.52
2	F	208	GLN	C-O	9.62	1.35	1.24
2	F	218	ASN	CA-C	9.55	1.67	1.52
2	B	102	VAL	CA-CB	9.48	1.67	1.54
1	E	80	GLU	CG-CD	9.48	1.75	1.52
2	H	100	GLY	CA-C	9.39	1.59	1.51
2	H	103	THR	CA-CB	9.35	1.69	1.53
2	B	192	ASN	N-CA	9.31	1.58	1.46
2	F	46	ALA	CA-C	9.28	1.65	1.52
1	C	83	THR	N-CA	9.12	1.56	1.45
2	D	22	GLY	C-O	8.88	1.36	1.23
1	E	19	VAL	CA-CB	8.80	1.65	1.54
2	B	173	GLU	C-O	8.79	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	LEU	C-O	-8.74	1.14	1.24
2	D	56	LYS	CA-C	8.68	1.64	1.52
1	C	71	SER	N-CA	8.67	1.56	1.45
1	A	69	ARG	CA-CB	-8.65	1.43	1.53
2	H	208	GLN	C-O	-8.61	1.14	1.24
1	G	46	ILE	CA-CB	8.60	1.64	1.54
1	A	78	ILE	CA-CB	-8.60	1.43	1.54
2	B	134	TYR	CA-C	-8.59	1.42	1.52
1	E	51	GLY	CA-C	8.58	1.60	1.51
2	D	209	SER	CA-C	-8.56	1.41	1.52
2	D	91	VAL	C-O	8.54	1.34	1.24
2	F	76	LYS	C-O	8.54	1.33	1.24
2	B	229	GLU	C-O	-8.51	1.12	1.23
2	B	25	LYS	N-CA	8.50	1.56	1.46
2	B	161	ALA	C-O	-8.48	1.14	1.24
2	B	27	LEU	C-O	8.47	1.34	1.24
1	A	33	TYR	CA-C	8.40	1.62	1.52
1	G	63	GLY	C-N	8.40	1.44	1.33
2	F	230	VAL	CA-CB	-8.40	1.44	1.54
2	B	87	SER	N-CA	-8.29	1.36	1.46
2	B	29	ASP	C-O	-8.28	1.13	1.23
2	D	141	ILE	CA-CB	8.24	1.64	1.55
2	B	67	GLU	CA-C	-8.23	1.42	1.52
1	A	47	HIS	C-O	-8.19	1.14	1.23
1	A	74	GLN	CA-C	-8.17	1.43	1.52
2	D	20	THR	CA-C	8.13	1.62	1.52
1	C	45	LEU	CA-C	-8.10	1.42	1.52
2	F	228	ILE	C-O	-8.10	1.15	1.24
2	D	158	ASP	N-CA	8.10	1.56	1.46
2	D	206	PHE	C-O	-8.07	1.15	1.24
1	A	37	GLN	N-CA	8.06	1.56	1.46
2	B	44	PHE	N-CA	7.97	1.54	1.46
2	D	146	GLN	N-CA	7.93	1.56	1.45
1	E	80	GLU	CA-CB	7.93	1.66	1.53
2	H	27	LEU	N-CA	7.91	1.56	1.46
2	D	172	TYR	C-O	7.89	1.33	1.24
1	C	76	SER	C-O	-7.84	1.14	1.23
1	G	100	LEU	C-O	-7.83	1.14	1.24
2	D	171	LEU	C-O	7.83	1.33	1.24
2	F	145	VAL	CA-CB	7.79	1.66	1.54
1	A	19	VAL	CA-C	7.74	1.61	1.52
1	C	43	LEU	C-O	-7.74	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	171	LEU	C-O	7.71	1.33	1.24
1	C	14	VAL	C-O	7.71	1.32	1.24
1	E	80	GLU	CA-C	7.70	1.63	1.52
1	C	12	VAL	CA-CB	-7.68	1.44	1.54
2	B	216	ASN	N-CA	7.67	1.55	1.46
2	F	50	ILE	CA-CB	7.66	1.64	1.54
2	B	214	MET	N-CA	-7.65	1.36	1.46
2	B	110	TYR	N-CA	7.64	1.55	1.46
1	E	54	SER	N-CA	7.64	1.55	1.46
2	F	30	ASP	C-O	-7.59	1.14	1.24
1	C	57	LYS	C-O	-7.58	1.14	1.24
2	F	200	PRO	C-O	7.57	1.33	1.24
1	G	66	LYS	CA-CB	-7.53	1.40	1.53
2	B	26	TYR	CB-CG	7.53	1.68	1.51
2	F	25	LYS	CA-C	7.52	1.62	1.52
1	A	51	GLY	N-CA	7.50	1.54	1.45
1	G	71	SER	N-CA	7.50	1.55	1.46
2	F	176	SER	N-CA	-7.48	1.40	1.46
1	E	91	PHE	N-CA	7.47	1.55	1.45
2	H	172	TYR	CE1-CZ	7.47	1.56	1.38
1	G	77	LEU	C-O	7.46	1.32	1.23
2	H	160	LYS	N-CA	7.43	1.55	1.46
2	H	184	ILE	CA-CB	7.43	1.63	1.53
2	F	91	VAL	C-O	7.41	1.32	1.24
2	B	28	TYR	N-CA	7.41	1.56	1.46
2	D	50	ILE	CA-CB	7.40	1.63	1.54
1	E	100	LEU	N-CA	7.39	1.54	1.45
1	E	61	PRO	N-CA	-7.39	1.39	1.47
2	D	62	ASP	CA-C	-7.37	1.43	1.52
1	E	62	ASP	C-O	7.33	1.32	1.23
1	A	79	LEU	CA-C	-7.33	1.44	1.52
2	D	201	ALA	CA-CB	-7.32	1.41	1.53
1	G	20	THR	C-O	7.30	1.32	1.24
2	B	74	ALA	CA-CB	-7.28	1.41	1.53
1	C	116	VAL	N-CA	-7.21	1.37	1.46
2	H	101	LYS	CA-CB	7.21	1.67	1.53
2	H	63	LYS	N-CA	-7.20	1.37	1.46
1	A	26	THR	CB-CG2	7.18	1.76	1.52
2	B	232	LEU	CA-C	-7.18	1.44	1.52
2	D	98	LYS	N-CA	7.18	1.55	1.46
1	A	32	MET	C-N	7.18	1.43	1.33
1	A	29	HIS	CA-C	-7.16	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	65	TYR	N-CA	7.16	1.55	1.45
1	C	53	GLY	N-CA	7.14	1.55	1.45
2	B	169	LYS	C-O	7.11	1.33	1.24
1	G	29	HIS	N-CA	7.10	1.55	1.45
1	E	89	VAL	CA-C	-7.10	1.44	1.52
2	F	141	ILE	CA-CB	7.08	1.64	1.54
2	F	75	LYS	CA-C	7.08	1.62	1.52
2	H	195	TRP	CA-C	7.06	1.61	1.52
1	G	108	PHE	C-O	7.06	1.33	1.23
2	B	145	VAL	CA-C	7.05	1.61	1.52
2	F	105	GLY	N-CA	7.05	1.52	1.45
1	G	56	GLU	CA-C	7.05	1.61	1.52
2	F	56	LYS	CA-C	7.03	1.61	1.52
2	H	165	LEU	CA-C	-7.02	1.43	1.52
2	F	226	VAL	CA-CB	7.02	1.61	1.54
1	A	53	GLY	CA-C	-7.01	1.42	1.52
2	B	42	ASP	CA-C	7.01	1.61	1.52
2	D	86	GLY	C-O	-7.01	1.16	1.24
2	H	210	LYS	CA-C	-7.00	1.43	1.52
2	H	41	VAL	N-CA	6.99	1.52	1.46
1	A	25	GLN	CD-NE2	6.99	1.48	1.33
2	H	54	SER	CA-C	6.99	1.61	1.52
2	B	88	ASN	CA-C	6.96	1.62	1.53
1	A	45	LEU	CA-C	-6.95	1.43	1.52
2	H	163	ASN	N-CA	6.94	1.55	1.46
1	C	46	ILE	CA-CB	-6.93	1.45	1.54
1	C	78	ILE	CG1-CD1	-6.91	1.24	1.51
1	E	67	ALA	N-CA	6.89	1.55	1.46
2	D	46	ALA	CA-CB	6.88	1.64	1.53
1	E	61	PRO	CA-C	6.88	1.60	1.52
2	H	218	ASN	CA-C	6.84	1.61	1.52
2	B	129	VAL	C-O	-6.83	1.16	1.24
1	E	6	GLN	N-CA	6.81	1.54	1.46
1	A	33	TYR	CD2-CE2	6.79	1.59	1.38
1	A	50	TYR	C-O	-6.79	1.14	1.24
2	H	75	LYS	N-CA	6.78	1.54	1.46
2	B	24	MET	C-N	6.77	1.42	1.33
1	A	91	PHE	C-O	-6.77	1.16	1.24
2	F	117	GLU	N-CA	6.74	1.54	1.46
2	F	171	LEU	C-O	6.73	1.32	1.24
1	C	77	LEU	N-CA	6.72	1.54	1.45
2	H	89	TYR	CA-C	-6.72	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	174	PHE	C-O	-6.71	1.16	1.24
2	D	67	GLU	CA-C	-6.70	1.44	1.52
2	H	25	LYS	C-O	-6.68	1.15	1.24
2	H	179	TYR	CA-C	-6.67	1.44	1.53
1	C	80	GLU	CG-CD	6.66	1.68	1.52
1	A	70	PRO	C-O	6.65	1.32	1.24
2	B	133	VAL	CA-CB	6.64	1.63	1.54
2	D	200	PRO	CA-C	-6.64	1.44	1.52
2	B	23	ASN	CA-CB	6.62	1.64	1.53
2	F	46	ALA	CA-CB	6.61	1.63	1.53
2	F	211	TYR	N-CA	6.61	1.54	1.46
1	A	76	SER	C-O	-6.61	1.16	1.24
2	F	176	SER	CA-C	6.60	1.57	1.53
2	H	46	ALA	CA-CB	6.60	1.64	1.53
2	F	142	SER	C-O	-6.59	1.15	1.23
1	A	56	GLU	CB-CG	6.58	1.72	1.52
1	E	116	VAL	CA-CB	6.57	1.62	1.54
2	D	235	LYS	N-CA	6.57	1.54	1.46
1	C	74	GLN	C-O	-6.57	1.16	1.24
2	F	161	ALA	CA-CB	6.55	1.64	1.53
2	F	32	TYR	CA-C	6.55	1.60	1.52
1	E	60	ILE	CA-CB	6.53	1.62	1.54
2	D	145	VAL	C-O	-6.52	1.16	1.23
1	E	67	ALA	CA-CB	6.51	1.64	1.53
2	H	163	ASN	C-O	-6.51	1.15	1.24
2	B	159	ILE	N-CA	-6.49	1.39	1.46
2	B	224	LYS	C-O	-6.48	1.15	1.24
2	H	36	THR	CA-C	6.48	1.60	1.52
2	H	157	LEU	C-O	6.47	1.32	1.24
2	B	220	THR	CA-CB	-6.46	1.40	1.54
2	F	65	LYS	C-O	6.45	1.31	1.24
2	H	137	LYS	CA-C	6.45	1.61	1.52
2	D	13	LYS	C-O	6.41	1.31	1.24
1	G	73	GLU	CA-C	-6.41	1.44	1.52
1	A	68	SER	C-O	-6.41	1.16	1.23
1	A	23	CYS	C-O	-6.40	1.16	1.24
2	B	231	HIS	CA-C	6.39	1.60	1.52
1	A	51	GLY	CA-C	6.39	1.58	1.51
2	F	109	MET	CA-C	-6.37	1.45	1.52
2	D	127	GLN	CA-C	6.37	1.61	1.52
2	F	20	THR	C-O	6.37	1.31	1.23
1	C	53	GLY	C-O	6.36	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	179	TYR	N-CA	-6.36	1.38	1.46
2	B	27	LEU	CA-CB	6.35	1.64	1.53
2	B	202	PRO	CA-C	6.35	1.60	1.52
1	A	74	GLN	CA-CB	-6.34	1.42	1.53
1	E	35	TYR	CA-C	6.34	1.60	1.52
2	H	159	ILE	CA-CB	-6.33	1.47	1.54
2	D	54	SER	CA-C	6.33	1.60	1.52
1	G	52	ALA	C-O	6.32	1.31	1.23
2	F	108	CYS	CA-C	6.32	1.60	1.52
2	D	98	LYS	CA-C	6.31	1.61	1.52
2	D	236	ASN	CA-C	6.31	1.61	1.52
1	A	83	THR	CA-C	6.31	1.60	1.52
1	C	84	PRO	N-CA	6.31	1.55	1.47
1	C	55	THR	C-O	6.31	1.31	1.24
1	E	110	ALA	N-CA	6.30	1.53	1.46
2	B	26	TYR	C-N	6.30	1.42	1.33
1	C	44	ARG	CA-C	6.30	1.61	1.53
1	C	55	THR	N-CA	6.29	1.54	1.46
1	G	83	THR	CA-C	-6.26	1.46	1.52
2	D	170	ASN	CA-C	-6.25	1.45	1.53
1	G	80	GLU	CG-CD	6.23	1.67	1.52
1	G	52	ALA	N-CA	6.23	1.54	1.46
1	G	15	THR	CA-CB	6.22	1.64	1.53
1	C	7	SER	CA-C	6.22	1.61	1.52
1	G	33	TYR	N-CA	6.22	1.53	1.46
1	C	115	SER	CA-C	-6.21	1.45	1.52
1	A	77	LEU	CA-C	-6.20	1.44	1.53
2	F	225	SER	C-O	6.20	1.31	1.23
1	G	3	ALA	N-CA	6.19	1.54	1.46
2	B	17	PHE	C-O	6.18	1.31	1.24
2	H	214	MET	CA-C	6.18	1.61	1.52
2	B	168	LYS	CA-C	6.17	1.61	1.52
1	E	101	TYR	CA-C	-6.17	1.46	1.53
1	G	5	THR	CA-C	-6.16	1.45	1.53
2	D	38	VAL	N-CA	6.16	1.53	1.46
2	B	28	TYR	C-O	6.15	1.31	1.23
2	H	35	ALA	CA-CB	-6.14	1.42	1.53
2	F	23	ASN	N-CA	6.14	1.54	1.46
2	H	103	THR	N-CA	6.14	1.54	1.46
2	B	166	ILE	CG1-CD1	-6.14	1.27	1.51
2	D	194	PHE	CA-C	-6.14	1.45	1.52
1	C	59	ASP	CA-C	-6.14	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ALA	C-O	-6.13	1.16	1.24
2	B	21	MET	N-CA	-6.13	1.38	1.46
2	F	84	VAL	CA-CB	6.13	1.61	1.54
1	G	35	TYR	N-CA	-6.13	1.38	1.45
2	D	102	VAL	N-CA	6.12	1.54	1.46
1	E	66	LYS	CA-C	6.12	1.61	1.53
1	E	14	VAL	CA-CB	6.11	1.61	1.54
1	A	62	ASP	C-O	6.10	1.31	1.24
2	F	145	VAL	C-O	-6.08	1.16	1.23
1	G	45	LEU	CA-CB	-6.08	1.45	1.53
2	D	43	LYS	CA-C	6.06	1.60	1.52
2	D	131	VAL	C-O	-6.05	1.17	1.24
2	F	58	LEU	N-CA	6.05	1.53	1.45
1	A	114	LEU	CA-C	-6.04	1.45	1.52
2	B	219	LYS	CG-CD	6.04	1.70	1.52
2	H	173	GLU	C-O	6.03	1.29	1.23
2	D	236	ASN	N-CA	6.03	1.53	1.46
2	F	91	VAL	CA-CB	6.03	1.62	1.54
2	B	85	TYR	C-O	-6.02	1.16	1.24
1	A	53	GLY	C-O	6.02	1.32	1.24
1	C	101	TYR	CA-C	-6.00	1.45	1.52
2	F	155	GLN	CA-C	6.00	1.60	1.52
1	G	91	PHE	C-O	5.99	1.31	1.24
1	C	79	LEU	CA-C	-5.99	1.45	1.52
2	H	154	ALA	CA-CB	5.98	1.63	1.53
2	B	223	SER	N-CA	5.97	1.53	1.46
2	D	65	LYS	C-O	5.97	1.30	1.24
2	F	107	THR	CA-CB	-5.97	1.44	1.53
1	E	52	ALA	CA-C	5.97	1.60	1.52
1	A	54	SER	CB-OG	5.96	1.54	1.42
1	E	45	LEU	CA-C	5.95	1.60	1.52
2	F	20	THR	CA-C	5.95	1.60	1.53
1	A	113	ARG	N-CA	5.94	1.53	1.46
2	B	127	GLN	C-O	-5.93	1.17	1.24
1	A	74	GLN	C-O	5.93	1.31	1.24
2	H	139	ASN	CA-C	5.93	1.60	1.52
2	D	113	ILE	N-CA	5.93	1.53	1.46
2	H	183	TYR	N-CA	5.93	1.53	1.45
2	H	31	HIS	C-O	5.92	1.30	1.23
2	F	151	SER	N-CA	5.92	1.53	1.46
1	A	55	THR	CB-CG2	5.92	1.72	1.52
2	B	219	LYS	CA-C	-5.92	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	133	VAL	CA-CB	5.92	1.62	1.54
1	C	66	LYS	CG-CD	5.91	1.70	1.52
2	F	65	LYS	N-CA	-5.90	1.39	1.46
2	B	216	ASN	CB-CG	-5.89	1.37	1.52
2	B	27	LEU	CB-CG	-5.88	1.41	1.53
2	D	65	LYS	CD-CE	5.88	1.70	1.52
1	A	75	PHE	CG-CD1	-5.85	1.26	1.38
2	D	172	TYR	CE2-CZ	5.85	1.52	1.38
2	H	17	PHE	N-CA	5.84	1.53	1.46
2	H	77	TYR	N-CA	5.84	1.53	1.46
2	D	153	THR	C-O	-5.83	1.17	1.23
1	A	77	LEU	N-CA	5.82	1.53	1.45
2	D	184	ILE	CA-CB	-5.82	1.46	1.54
2	B	28	TYR	CA-C	5.81	1.60	1.52
1	C	94	SER	N-CA	-5.81	1.38	1.45
2	H	201	ALA	CA-CB	5.81	1.62	1.53
2	D	235	LYS	CA-C	5.80	1.60	1.52
1	G	27	ASN	C-O	5.80	1.31	1.24
1	C	32	MET	N-CA	5.79	1.53	1.45
2	H	11	LEU	CA-C	-5.79	1.45	1.52
2	H	64	VAL	CA-CB	5.78	1.61	1.54
1	E	34	TRP	CA-CB	5.78	1.62	1.53
2	D	114	THR	CA-C	5.77	1.59	1.52
2	F	164	PHE	CA-C	5.77	1.60	1.52
2	B	30	ASP	CA-C	-5.77	1.45	1.52
2	B	63	LYS	CD-CE	5.76	1.69	1.52
1	G	20	THR	CA-CB	5.75	1.62	1.53
1	A	36	ARG	N-CA	5.75	1.52	1.45
2	F	37	LYS	N-CA	5.72	1.53	1.46
2	F	42	ASP	C-O	-5.71	1.16	1.24
2	F	11	LEU	N-CA	5.70	1.52	1.46
2	B	205	LYS	CD-CE	5.70	1.69	1.52
1	C	92	CYS	N-CA	-5.69	1.38	1.45
2	H	62	ASP	C-O	-5.69	1.19	1.23
1	G	71	SER	C-O	5.68	1.30	1.23
1	A	90	TYR	C-O	5.67	1.30	1.24
2	B	165	LEU	N-CA	5.67	1.53	1.46
2	D	76	LYS	C-O	5.67	1.31	1.24
2	F	236	ASN	CA-C	5.66	1.60	1.52
1	G	67	ALA	CA-C	-5.66	1.45	1.52
2	H	52	ASN	N-CA	-5.66	1.39	1.46
1	A	30	ASN	CB-CG	5.65	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	56	LYS	CA-CB	5.65	1.60	1.53
2	F	216	ASN	C-O	5.64	1.31	1.24
2	F	168	LYS	N-CA	5.64	1.53	1.46
2	B	22	GLY	N-CA	5.64	1.54	1.45
2	B	174	PHE	CE1-CZ	-5.64	1.21	1.38
1	A	18	LYS	C-O	-5.62	1.17	1.24
1	G	37	GLN	C-O	-5.61	1.16	1.23
1	G	51	GLY	CA-C	5.61	1.58	1.52
1	A	14	VAL	N-CA	5.61	1.53	1.46
2	H	145	VAL	CA-CB	-5.61	1.46	1.54
2	H	228	ILE	C-O	-5.61	1.18	1.24
2	B	164	PHE	CE1-CZ	5.59	1.55	1.38
1	A	112	THR	CA-CB	5.59	1.62	1.53
2	H	26	TYR	N-CA	5.59	1.53	1.46
2	B	159	ILE	CA-C	5.59	1.59	1.52
1	C	74	GLN	CA-CB	-5.59	1.45	1.53
2	D	186	PHE	N-CA	5.59	1.53	1.46
2	B	51	TYR	C-O	-5.58	1.16	1.23
1	A	29	HIS	N-CA	-5.57	1.39	1.46
2	B	27	LEU	CG-CD2	5.57	1.71	1.52
2	H	100	GLY	N-CA	5.57	1.51	1.45
2	F	57	LYS	N-CA	5.56	1.53	1.46
1	A	101	TYR	C-O	-5.56	1.17	1.24
1	A	93	ALA	C-O	5.56	1.30	1.24
2	F	209	SER	CA-C	-5.56	1.45	1.52
2	H	68	LEU	CA-C	-5.55	1.45	1.53
2	D	28	TYR	CA-C	5.54	1.59	1.52
2	H	186	PHE	C-O	5.52	1.30	1.23
2	F	203	GLY	CA-C	-5.51	1.45	1.52
1	G	19	VAL	CA-CB	5.51	1.62	1.54
2	B	165	LEU	CA-C	-5.50	1.45	1.52
1	G	89	VAL	C-O	5.50	1.31	1.24
2	B	94	TYR	N-CA	-5.50	1.39	1.46
1	E	48	TYR	N-CA	5.50	1.53	1.46
2	D	205	LYS	CG-CD	5.49	1.69	1.52
2	B	41	VAL	CA-C	5.49	1.60	1.52
1	C	43	LEU	CA-C	-5.48	1.46	1.52
2	D	228	ILE	CA-CB	-5.48	1.46	1.54
2	D	210	LYS	N-CA	-5.47	1.39	1.46
2	H	208	GLN	CA-C	-5.47	1.45	1.52
2	D	209	SER	C-O	-5.47	1.17	1.24
2	D	24	MET	N-CA	5.46	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	15	THR	CA-CB	-5.46	1.44	1.53
2	H	213	MET	CA-C	5.46	1.60	1.52
2	D	160	LYS	C-O	5.46	1.30	1.23
2	F	233	THR	CA-CB	5.46	1.65	1.53
1	G	59	ASP	CG-OD1	5.46	1.35	1.25
2	B	25	LYS	CG-CD	5.45	1.68	1.52
2	H	113	ILE	C-O	5.45	1.30	1.24
1	C	92	CYS	C-O	5.45	1.30	1.23
2	F	200	PRO	CA-C	5.45	1.60	1.52
2	B	32	TYR	N-CA	5.44	1.53	1.46
2	D	95	PHE	N-CA	-5.44	1.39	1.47
2	B	23	ASN	CA-C	5.44	1.59	1.52
2	D	21	MET	C-O	5.43	1.31	1.24
2	D	194	PHE	C-O	-5.42	1.17	1.23
1	E	116	VAL	N-CA	5.42	1.52	1.46
2	F	75	LYS	N-CA	5.41	1.53	1.46
1	A	32	MET	N-CA	5.40	1.52	1.45
2	B	90	TYR	N-CA	5.40	1.53	1.46
2	D	5	ASP	CG-OD1	5.40	1.35	1.25
1	C	55	THR	CB-OG1	5.39	1.52	1.43
2	F	104	GLY	C-N	5.38	1.37	1.33
1	G	100	LEU	N-CA	5.38	1.52	1.46
2	H	166	ILE	CA-CB	5.38	1.61	1.54
2	D	159	ILE	CA-CB	5.37	1.60	1.54
2	H	156	GLU	C-O	-5.37	1.17	1.24
2	F	144	GLU	CA-C	5.37	1.59	1.52
2	B	103	THR	CA-CB	5.37	1.62	1.53
2	F	115	LYS	CB-CG	5.37	1.68	1.52
1	C	39	THR	CA-CB	5.36	1.62	1.53
1	G	95	GLY	N-CA	5.36	1.51	1.45
1	E	3	ALA	N-CA	5.35	1.53	1.46
1	C	80	GLU	CD-OE2	5.35	1.35	1.25
2	F	172	TYR	CA-C	-5.35	1.46	1.52
2	B	131	VAL	C-O	5.33	1.30	1.24
2	D	23	ASN	N-CA	5.33	1.52	1.46
2	B	77	TYR	CA-C	-5.33	1.45	1.52
2	B	185	LYS	C-O	5.33	1.30	1.24
1	G	65	TYR	CE2-CZ	5.32	1.51	1.38
2	D	162	ARG	CG-CD	5.32	1.68	1.52
2	H	67	GLU	N-CA	-5.31	1.40	1.46
2	D	157	LEU	CG-CD1	-5.31	1.35	1.52
2	B	228	ILE	C-O	5.31	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	126	LEU	CA-C	-5.30	1.45	1.52
2	H	158	ASP	C-O	5.30	1.30	1.24
1	E	22	SER	C-O	-5.29	1.17	1.23
1	C	47	HIS	CA-C	5.29	1.58	1.52
2	D	232	LEU	C-O	-5.29	1.18	1.24
1	C	112	THR	CA-C	-5.27	1.46	1.52
1	A	99	THR	CA-C	5.27	1.59	1.52
1	A	98	GLY	C-O	-5.26	1.17	1.24
2	D	14	SER	N-CA	-5.26	1.39	1.46
2	H	164	PHE	CA-CB	5.26	1.61	1.53
2	H	221	VAL	C-O	5.26	1.30	1.24
2	D	162	ARG	CZ-NH2	5.25	1.40	1.33
1	E	20	THR	CA-CB	5.25	1.61	1.53
2	B	24	MET	CA-CB	5.24	1.62	1.53
1	G	84	PRO	CA-C	5.23	1.61	1.52
1	A	27	ASN	CG-OD1	5.23	1.33	1.23
2	D	147	THR	C-O	-5.23	1.18	1.24
1	C	51	GLY	C-O	5.23	1.31	1.23
1	G	95	GLY	C-O	-5.23	1.17	1.23
1	E	3	ALA	CA-C	5.22	1.59	1.52
2	D	211	TYR	CA-C	5.22	1.60	1.52
1	C	114	LEU	N-CA	-5.22	1.39	1.45
1	A	50	TYR	CA-C	-5.22	1.45	1.52
2	B	115	LYS	CA-C	5.21	1.59	1.52
2	H	151	SER	CA-CB	5.21	1.59	1.53
1	A	39	THR	CA-CB	5.21	1.62	1.53
2	B	129	VAL	CA-CB	5.20	1.60	1.54
1	C	38	ASP	CB-CG	5.20	1.65	1.52
1	G	53	GLY	N-CA	-5.20	1.38	1.45
2	D	83	ASP	CA-C	5.19	1.58	1.52
2	B	83	ASP	C-O	5.19	1.30	1.23
1	E	57	LYS	CE-NZ	5.18	1.64	1.49
2	H	116	HIS	C-O	5.18	1.29	1.23
1	A	30	ASN	C-O	5.18	1.30	1.24
2	D	154	ALA	CA-CB	5.18	1.62	1.53
1	E	86	GLN	CA-C	-5.18	1.46	1.52
2	B	26	TYR	CG-CD2	5.17	1.50	1.39
2	H	192	ASN	CA-C	5.17	1.59	1.52
2	B	200	PRO	CA-C	5.16	1.58	1.52
1	G	31	ASN	CG-OD1	-5.16	1.13	1.23
2	D	184	ILE	CB-CG1	5.16	1.63	1.53
2	D	115	LYS	CG-CD	5.15	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	SER	C-O	5.15	1.30	1.24
1	E	79	LEU	CA-C	5.14	1.59	1.52
2	H	82	VAL	CB-CG1	5.14	1.69	1.52
2	B	210	LYS	C-O	5.14	1.30	1.24
1	C	94	SER	CA-C	5.14	1.58	1.52
2	D	183	TYR	N-CA	5.14	1.52	1.45
1	G	86	GLN	N-CA	5.14	1.52	1.46
2	B	89	TYR	CZ-OH	-5.14	1.27	1.38
2	B	206	PHE	CA-C	5.14	1.58	1.52
2	B	50	ILE	CA-CB	5.13	1.61	1.54
2	H	35	ALA	CA-C	-5.13	1.46	1.52
1	A	27	ASN	N-CA	-5.13	1.40	1.46
1	G	80	GLU	CD-OE2	5.13	1.35	1.25
1	G	88	SER	CA-C	-5.13	1.46	1.52
2	H	163	ASN	CA-C	-5.12	1.46	1.52
2	B	97	SER	CA-C	5.12	1.59	1.52
1	A	43	LEU	N-CA	5.12	1.52	1.46
2	F	56	LYS	N-CA	5.12	1.52	1.46
2	D	95	PHE	C-O	5.11	1.28	1.23
2	D	172	TYR	CD1-CE1	5.11	1.53	1.38
2	F	219	LYS	N-CA	5.11	1.52	1.46
1	G	62	ASP	CA-C	-5.11	1.46	1.52
1	A	5	THR	C-O	-5.10	1.17	1.24
2	F	89	TYR	CA-C	5.10	1.58	1.52
2	B	154	ALA	CA-C	5.09	1.59	1.52
1	A	66	LYS	CA-CB	-5.09	1.46	1.53
2	H	175	ASN	CB-CG	5.09	1.64	1.52
1	A	87	THR	CA-CB	5.08	1.61	1.53
1	E	93	ALA	CA-C	5.08	1.58	1.52
2	F	107	THR	CA-C	5.07	1.59	1.52
1	G	111	GLY	C-O	5.07	1.29	1.23
1	C	19	VAL	N-CA	5.07	1.52	1.46
2	B	218	ASN	CA-C	-5.06	1.45	1.52
1	G	31	ASN	CA-CB	-5.06	1.46	1.53
1	G	70	PRO	N-CA	-5.05	1.40	1.47
2	B	160	LYS	CA-CB	-5.05	1.45	1.53
1	E	99	THR	CA-C	5.05	1.59	1.52
2	F	134	TYR	CA-C	-5.05	1.46	1.52
2	H	177	SER	CA-CB	-5.05	1.47	1.54
2	B	209	SER	N-CA	5.05	1.52	1.46
2	B	232	LEU	CG-CD1	5.04	1.69	1.52
2	F	127	GLN	CA-C	5.03	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	58	GLY	N-CA	5.03	1.52	1.45
2	F	162	ARG	CG-CD	5.03	1.67	1.52
2	B	180	GLU	N-CA	-5.03	1.39	1.46
1	G	86	GLN	C-O	5.03	1.30	1.24
2	D	214	MET	N-CA	-5.02	1.40	1.46
2	B	147	THR	C-O	-5.02	1.17	1.23
2	F	98	LYS	CA-C	5.02	1.57	1.52
1	A	20	THR	CB-CG2	5.01	1.69	1.52
1	E	50	TYR	CZ-OH	5.01	1.48	1.38
1	C	46	ILE	N-CA	-5.01	1.40	1.46
2	B	188	GLU	CA-C	5.01	1.59	1.52
2	B	206	PHE	C-O	5.01	1.29	1.24
2	F	170	ASN	N-CA	5.00	1.53	1.46

All (477) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	101	TYR	O-C-N	-29.52	84.44	122.82
1	A	101	TYR	O-C-N	-26.52	87.32	122.59
1	E	101	TYR	O-C-N	-22.20	92.88	123.06
1	G	111	GLY	N-CA-C	12.71	128.69	112.68
2	D	149	LYS	N-CA-C	-11.98	90.58	109.50
2	B	23	ASN	N-CA-C	-11.86	98.30	113.12
2	F	201	ALA	CA-C-N	11.29	131.25	119.85
2	F	201	ALA	C-N-CA	11.29	131.25	119.85
2	D	60	ASN	N-CA-C	11.10	125.97	113.21
1	C	69	ARG	CA-C-N	-11.04	107.49	119.19
1	C	69	ARG	C-N-CA	-11.04	107.49	119.19
1	E	60	ILE	CA-C-N	-10.93	107.66	120.89
1	E	60	ILE	C-N-CA	-10.93	107.66	120.89
2	F	120	HIS	N-CA-C	10.89	125.38	110.35
2	B	199	MET	CA-C-N	-10.57	108.93	120.14
2	B	199	MET	C-N-CA	-10.57	108.93	120.14
2	B	217	ASP	N-CA-C	-10.50	100.47	113.28
1	A	77	LEU	CA-C-O	-10.38	109.83	121.87
2	B	167	ASN	N-CA-C	-10.38	97.32	111.96
1	C	60	ILE	CA-C-N	10.38	130.13	119.64
1	C	60	ILE	C-N-CA	10.38	130.13	119.64
2	B	88	ASN	N-CA-C	10.22	124.35	110.55
2	F	76	LYS	N-CA-C	10.14	121.92	111.07
1	G	50	TYR	N-CA-C	10.10	124.83	113.21
1	E	110	ALA	N-CA-C	10.06	123.64	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	LYS	N-CA-C	9.69	124.16	111.75
2	B	24	MET	N-CA-C	9.47	130.98	110.80
1	E	63	GLY	O-C-N	-9.47	110.39	122.70
2	H	52	ASN	CB-CA-C	-9.46	96.78	112.00
1	E	101	TYR	CA-C-N	-9.39	104.27	122.02
1	E	101	TYR	C-N-CA	-9.39	104.27	122.02
1	A	68	SER	N-CA-C	9.25	124.03	108.13
2	D	162	ARG	NE-CZ-NH1	-9.25	112.25	121.50
1	G	37	GLN	N-CA-C	9.09	123.87	108.23
2	B	5	ASP	CA-C-N	9.06	129.14	119.90
2	B	5	ASP	C-N-CA	9.06	129.14	119.90
1	A	77	LEU	N-CA-C	-9.01	98.64	110.53
2	H	58	LEU	N-CA-C	-9.00	94.49	109.80
1	G	57	LYS	N-CA-C	8.97	122.18	110.43
2	B	14	SER	N-CA-C	-8.96	101.59	111.36
1	G	95	GLY	N-CA-C	8.93	124.56	110.90
2	B	9	ASP	N-CA-C	-8.80	102.95	114.31
2	B	124	GLY	N-CA-C	-8.73	102.54	115.72
2	B	27	LEU	N-CA-C	-8.72	102.54	113.01
2	D	192	ASN	N-CA-C	8.72	123.09	110.10
2	B	213	MET	N-CA-C	-8.67	102.14	112.89
1	G	69	ARG	CA-C-N	8.63	129.16	119.32
1	G	69	ARG	C-N-CA	8.63	129.16	119.32
1	A	36	ARG	N-CA-C	8.60	123.47	110.14
1	E	53	GLY	N-CA-C	8.60	126.39	115.21
2	F	24	MET	CG-SD-CE	-8.38	82.47	100.90
1	G	99	THR	CB-CA-C	-8.37	97.71	110.26
2	D	173	GLU	N-CA-C	8.36	121.73	109.69
2	B	173	GLU	N-CA-C	8.34	121.96	109.95
2	H	112	GLY	N-CA-C	8.24	127.16	115.30
2	F	225	SER	N-CA-C	8.15	124.41	113.97
1	C	52	ALA	O-C-N	-8.10	113.00	122.89
2	D	113	ILE	CB-CA-C	-8.06	98.69	110.63
1	C	115	SER	CA-C-N	-8.05	112.97	122.95
1	C	115	SER	C-N-CA	-8.05	112.97	122.95
2	D	145	VAL	CA-C-O	-7.99	113.45	120.96
2	F	144	GLU	N-CA-C	7.99	122.42	109.40
1	G	99	THR	N-CA-C	7.99	121.33	109.59
1	E	90	TYR	CA-C-O	-7.94	112.13	120.70
2	D	28	TYR	N-CA-C	7.91	124.09	113.97
2	B	145	VAL	CB-CA-C	7.88	122.96	110.82
2	B	192	ASN	N-CA-C	7.83	121.85	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	TYR	O-C-N	-7.80	113.09	122.22
2	D	224	LYS	N-CA-C	7.76	122.43	112.34
2	B	211	TYR	CA-C-N	-7.75	109.23	122.56
2	B	211	TYR	C-N-CA	-7.75	109.23	122.56
2	B	216	ASN	CB-CA-C	-7.65	98.03	110.74
1	A	94	SER	N-CA-C	-7.65	98.62	110.17
1	A	77	LEU	O-C-N	7.63	131.49	122.79
2	B	164	PHE	N-CA-C	7.63	120.27	111.11
2	B	196	TYR	CA-C-N	7.61	132.28	121.02
2	B	196	TYR	C-N-CA	7.61	132.28	121.02
1	C	97	GLY	N-CA-C	-7.59	95.19	113.18
2	D	90	TYR	N-CA-C	-7.58	94.65	110.80
2	D	213	MET	N-CA-C	-7.58	104.00	113.18
1	A	74	GLN	CB-CA-C	-7.58	95.75	109.38
2	B	230	VAL	N-CA-C	-7.57	96.50	107.78
2	D	15	SER	N-CA-C	-7.55	104.17	113.15
2	B	215	TYR	N-CA-C	-7.49	103.70	112.92
2	D	229	GLU	CA-C-N	-7.49	113.91	123.19
2	D	229	GLU	C-N-CA	-7.49	113.91	123.19
1	A	28	ASN	CA-C-N	-7.47	112.69	123.00
1	A	28	ASN	C-N-CA	-7.47	112.69	123.00
2	F	167	ASN	N-CA-C	7.44	120.27	111.71
2	H	189	ASN	N-CA-C	-7.42	104.20	113.18
2	F	179	TYR	N-CA-C	7.41	121.77	109.46
2	D	174	PHE	N-CA-C	-7.39	103.15	111.14
1	A	109	GLY	N-CA-C	-7.35	101.38	112.41
1	A	26	THR	N-CA-C	-7.33	104.19	113.72
2	H	171	LEU	N-CA-C	-7.30	103.35	111.82
1	G	80	GLU	N-CA-C	-7.30	104.51	113.19
2	H	226	VAL	N-CA-C	7.30	124.52	109.34
2	B	36	THR	CB-CA-C	-7.29	98.23	110.19
1	C	23	CYS	CB-CA-C	7.28	121.34	110.14
2	F	7	MET	N-CA-C	-7.26	99.47	110.50
2	F	7	MET	CA-C-N	7.25	128.90	119.84
2	F	7	MET	C-N-CA	7.25	128.90	119.84
1	G	53	GLY	N-CA-C	7.22	125.37	114.61
2	B	132	ARG	N-CA-C	7.21	121.59	109.76
1	C	79	LEU	CB-CG-CD1	7.21	132.31	110.70
1	G	83	THR	CA-C-N	-7.20	111.12	119.47
1	G	83	THR	C-N-CA	-7.20	111.12	119.47
1	G	55	THR	CB-CA-C	-7.19	98.01	109.80
2	D	209	SER	N-CA-C	-7.18	103.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	163	ASN	N-CA-C	7.18	118.79	110.97
1	A	92	CYS	CA-CB-SG	-7.16	97.94	114.40
1	G	60	ILE	N-CA-C	7.14	124.30	108.88
2	B	63	LYS	CA-C-N	-7.12	113.92	123.10
2	B	63	LYS	C-N-CA	-7.12	113.92	123.10
1	G	29	HIS	N-CA-CB	7.11	121.41	110.60
1	A	97	GLY	N-CA-C	-7.08	102.86	111.35
1	A	108	PHE	CA-C-N	-7.07	115.27	122.27
1	A	108	PHE	C-N-CA	-7.07	115.27	122.27
2	D	17	PHE	CA-C-N	-7.07	111.49	122.37
2	D	17	PHE	C-N-CA	-7.07	111.49	122.37
2	H	147	THR	CB-CA-C	-7.03	94.59	110.07
1	E	96	GLY	N-CA-C	-6.96	98.91	111.15
2	D	53	ILE	N-CA-C	-6.95	98.16	108.45
2	B	47	HIS	N-CA-C	6.93	121.19	113.21
2	F	109	MET	N-CA-C	-6.88	99.79	108.45
1	C	32	MET	CB-CG-SD	6.87	133.30	112.70
2	D	37	LYS	N-CA-C	6.86	118.94	110.91
1	C	7	SER	N-CA-C	6.82	118.25	109.72
1	A	50	TYR	CA-C-O	-6.82	111.54	119.59
2	D	88	ASN	CB-CA-C	6.81	122.38	109.37
1	G	101	TYR	CB-CA-C	-6.80	101.76	111.76
2	H	91	VAL	CB-CA-C	6.80	118.58	111.23
1	G	45	LEU	CA-C-N	6.80	129.01	120.72
1	G	45	LEU	C-N-CA	6.80	129.01	120.72
2	B	22	GLY	N-CA-C	-6.79	107.20	114.67
2	F	172	TYR	N-CA-C	-6.78	96.69	108.69
2	B	99	ASP	N-CA-C	-6.77	102.09	112.99
1	G	40	GLY	N-CA-C	6.75	121.68	113.79
2	H	72	ASP	CB-CA-C	-6.74	100.58	110.96
2	F	170	ASN	N-CA-CB	6.73	122.28	111.65
2	D	129	VAL	CA-C-N	-6.70	113.47	122.72
2	D	129	VAL	C-N-CA	-6.70	113.47	122.72
2	F	106	LYS	N-CA-C	6.70	119.31	108.32
1	A	44	ARG	N-CA-C	6.70	120.15	109.24
2	F	117	GLU	CB-CA-C	-6.69	101.57	109.80
2	F	158	ASP	N-CA-C	-6.68	103.92	111.14
2	B	161	ALA	N-CA-C	-6.65	103.29	111.40
1	E	26	THR	N-CA-C	6.62	121.57	112.90
1	A	29	HIS	N-CA-C	-6.61	98.43	109.07
1	G	96	GLY	N-CA-C	-6.61	97.52	113.18
1	G	51	GLY	CA-C-O	-6.60	116.99	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	172	TYR	N-CA-C	-6.60	96.13	107.61
2	H	167	ASN	N-CA-C	6.59	119.03	111.11
2	F	33	VAL	CB-CA-C	-6.56	101.73	110.98
1	A	60	ILE	CA-C-N	-6.56	111.64	119.84
1	A	60	ILE	C-N-CA	-6.56	111.64	119.84
1	C	89	VAL	CB-CA-C	-6.56	100.85	110.62
2	H	81	VAL	N-CA-C	-6.55	100.30	109.21
1	A	25	GLN	CA-C-N	-6.54	111.86	122.26
1	A	25	GLN	C-N-CA	-6.54	111.86	122.26
2	H	128	ASN	CB-CA-C	-6.53	98.49	109.53
1	A	52	ALA	CA-C-N	-6.53	115.68	123.44
1	A	52	ALA	C-N-CA	-6.53	115.68	123.44
1	C	22	SER	N-CA-C	6.52	120.13	110.48
2	B	212	LEU	N-CA-C	-6.52	105.20	113.02
1	C	76	SER	N-CA-CB	-6.50	100.37	111.69
1	E	90	TYR	N-CA-C	-6.49	98.83	109.40
1	G	79	LEU	CA-CB-CG	6.48	138.97	116.30
2	D	26	TYR	N-CA-C	-6.47	103.73	111.69
1	E	63	GLY	CA-C-N	-6.46	112.53	122.09
1	E	63	GLY	C-N-CA	-6.46	112.53	122.09
2	B	196	TYR	CA-CB-CG	6.46	125.52	113.90
2	D	95	PHE	N-CA-C	6.45	118.57	107.28
2	B	25	LYS	O-C-N	-6.44	114.70	122.11
2	H	41	VAL	CB-CA-C	6.44	117.57	110.62
2	B	104	GLY	CA-C-N	6.43	126.87	120.31
2	B	104	GLY	C-N-CA	6.43	126.87	120.31
2	D	33	VAL	CB-CA-C	-6.40	102.45	111.21
2	H	162	ARG	N-CA-C	-6.40	103.82	111.69
2	D	73	LEU	N-CA-C	-6.37	97.23	110.80
2	B	231	HIS	N-CA-C	6.36	119.25	107.99
2	F	72	ASP	N-CA-C	-6.36	104.28	111.14
2	F	156	GLU	O-C-N	-6.36	115.48	122.09
2	H	10	ASP	N-CA-C	6.34	119.95	112.72
1	E	74	GLN	N-CA-C	6.33	119.89	108.69
1	A	111	GLY	CA-C-N	-6.31	113.90	122.86
1	A	111	GLY	C-N-CA	-6.31	113.90	122.86
2	H	233	THR	CB-CA-C	-6.30	103.61	111.43
2	H	177	SER	CA-C-N	-6.29	114.41	120.83
2	H	177	SER	C-N-CA	-6.29	114.41	120.83
2	B	131	VAL	N-CA-C	6.29	116.92	107.80
1	C	108	PHE	N-CA-C	6.29	119.61	109.86
1	A	36	ARG	NE-CZ-NH2	6.29	124.86	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	LYS	CG-CD-CE	-6.29	96.83	111.30
2	D	233	THR	CB-CA-C	-6.29	99.58	110.45
1	A	93	ALA	N-CA-C	-6.28	97.42	110.80
1	G	32	MET	N-CA-C	-6.28	99.58	109.50
2	D	145	VAL	N-CA-C	-6.27	100.03	108.06
2	B	165	LEU	CB-CG-CD2	-6.24	92.00	110.70
2	B	232	LEU	CA-C-O	-6.24	114.06	121.11
2	D	38	VAL	N-CA-C	6.24	117.75	108.46
1	G	101	TYR	CA-C-N	6.24	134.79	121.45
1	G	101	TYR	C-N-CA	6.24	134.79	121.45
2	B	216	ASN	N-CA-C	6.21	121.61	111.37
1	G	75	PHE	CA-C-N	-6.19	112.96	122.62
1	G	75	PHE	C-N-CA	-6.19	112.96	122.62
1	A	36	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	C	20	THR	CA-C-N	-6.16	114.31	123.00
1	C	20	THR	C-N-CA	-6.16	114.31	123.00
2	D	76	LYS	N-CA-C	6.14	119.87	112.38
2	F	145	VAL	O-C-N	-6.14	116.98	122.69
1	C	92	CYS	N-CA-C	-6.14	99.80	109.50
2	B	123	ASN	N-CA-C	6.13	122.09	113.56
2	H	165	LEU	N-CA-C	-6.13	105.63	113.23
1	C	83	THR	CB-CA-C	6.12	118.36	108.87
2	F	142	SER	CA-C-N	-6.10	111.98	122.10
2	F	142	SER	C-N-CA	-6.10	111.98	122.10
2	H	26	TYR	CA-C-N	6.09	133.16	121.54
2	H	26	TYR	C-N-CA	6.09	133.16	121.54
2	F	125	ASN	N-CA-C	6.08	118.17	110.33
1	A	33	TYR	CA-C-O	-6.08	114.01	121.06
1	C	55	THR	N-CA-CB	6.07	120.75	110.49
1	A	32	MET	N-CA-CB	-6.07	101.97	111.56
2	H	188	GLU	CA-C-N	-6.06	109.76	121.58
2	H	188	GLU	C-N-CA	-6.06	109.76	121.58
2	H	207	ASP	N-CA-C	6.06	119.37	107.98
2	D	175	ASN	CB-CA-C	6.05	118.83	109.03
2	B	209	SER	CA-C-N	6.05	128.30	120.44
2	B	209	SER	C-N-CA	6.05	128.30	120.44
1	A	22	SER	CB-CA-C	-6.04	99.84	109.80
1	E	50	TYR	N-CA-C	6.04	120.35	112.92
2	F	236	ASN	N-CA-C	6.04	123.66	110.80
1	C	39	THR	N-CA-CB	6.02	118.81	109.97
2	B	93	CYS	N-CA-C	-6.01	98.49	108.34
1	C	88	SER	CA-C-N	5.99	131.33	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	SER	C-N-CA	5.99	131.33	123.06
1	E	3	ALA	N-CA-C	5.99	121.33	113.30
1	E	89	VAL	N-CA-C	-5.99	99.43	108.17
2	F	187	ILE	CB-CA-C	5.98	121.09	111.29
2	H	124	GLY	N-CA-C	-5.96	107.20	113.58
2	D	215	TYR	CA-C-N	5.96	128.55	120.38
2	D	215	TYR	C-N-CA	5.96	128.55	120.38
2	D	214	MET	CG-SD-CE	-5.96	87.79	100.90
2	F	170	ASN	CB-CA-C	-5.96	102.92	112.09
1	C	57	LYS	CB-CA-C	-5.95	100.14	109.84
2	D	25	LYS	N-CA-C	5.95	123.46	110.80
1	A	27	ASN	CA-C-N	5.94	132.89	121.54
1	A	27	ASN	C-N-CA	5.94	132.89	121.54
2	D	209	SER	O-C-N	5.94	128.93	122.15
2	B	222	ASP	N-CA-C	-5.94	98.85	108.41
2	H	192	ASN	N-CA-C	5.94	118.95	110.10
2	D	163	ASN	CA-C-N	5.93	128.55	120.54
2	D	163	ASN	C-N-CA	5.93	128.55	120.54
2	B	107	THR	CA-CB-OG1	-5.92	100.72	109.60
1	E	50	TYR	CA-CB-CG	5.90	124.53	113.90
1	C	75	PHE	CB-CA-C	-5.90	99.33	109.65
1	C	76	SER	CA-CB-OG	-5.89	99.31	111.10
2	D	91	VAL	N-CA-CB	5.89	120.95	111.23
2	D	202	PRO	CA-C-N	-5.89	114.19	122.85
2	D	202	PRO	C-N-CA	-5.89	114.19	122.85
2	B	113	ILE	N-CA-C	5.89	116.41	108.17
1	C	71	SER	CA-CB-OG	5.85	122.80	111.10
2	F	168	LYS	N-CA-C	5.84	120.53	113.41
2	D	162	ARG	NE-CZ-NH2	5.84	124.45	119.20
2	F	193	THR	N-CA-C	5.84	119.87	107.67
2	D	48	ASP	N-CA-C	5.83	119.07	109.85
1	C	70	PRO	CB-CA-C	-5.83	103.60	112.11
1	A	31	ASN	CB-CA-C	-5.82	99.92	109.53
2	B	125	ASN	N-CA-C	-5.82	101.87	110.48
2	D	50	ILE	CB-CA-C	-5.81	102.17	110.83
1	A	67	ALA	CA-C-N	-5.80	112.70	121.86
1	A	67	ALA	C-N-CA	-5.80	112.70	121.86
2	D	179	TYR	N-CA-CB	-5.80	101.92	110.85
2	H	223	SER	CA-C-N	5.79	128.04	120.28
2	H	223	SER	C-N-CA	5.79	128.04	120.28
1	E	80	GLU	CB-CG-CD	5.79	122.44	112.60
2	B	152	VAL	N-CA-C	-5.79	100.14	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	151	SER	N-CA-C	-5.79	99.76	108.96
2	H	106	LYS	CB-CA-C	-5.79	101.79	110.24
2	D	22	GLY	CA-C-N	5.79	128.50	120.29
2	D	22	GLY	C-N-CA	5.79	128.50	120.29
1	C	59	ASP	N-CA-C	-5.78	106.36	113.41
1	C	76	SER	O-C-N	-5.78	116.17	123.17
1	G	76	SER	N-CA-C	5.78	118.63	109.50
2	D	104	GLY	N-CA-C	-5.77	100.06	111.31
2	H	38	VAL	N-CA-C	5.76	117.01	108.65
2	F	145	VAL	N-CA-C	5.75	117.46	109.29
2	H	33	VAL	CB-CA-C	-5.75	103.02	110.84
2	H	214	MET	N-CA-C	5.75	119.40	112.38
2	D	171	LEU	O-C-N	5.75	128.06	122.09
2	H	159	ILE	N-CA-C	-5.74	105.02	110.42
1	A	94	SER	CA-C-O	-5.74	114.42	121.88
2	F	191	GLY	N-CA-C	-5.74	108.25	115.08
1	G	100	LEU	N-CA-C	5.73	118.88	109.76
2	B	92	ASN	N-CA-CB	5.73	120.17	110.49
2	B	185	LYS	N-CA-C	5.72	118.57	109.24
2	D	72	ASP	N-CA-C	-5.72	98.61	110.80
1	E	97	GLY	N-CA-C	5.72	126.74	113.18
1	C	18	LYS	CB-CA-C	5.72	119.19	109.53
1	C	79	LEU	N-CA-C	-5.72	98.97	108.34
2	H	47	HIS	N-CA-C	5.72	120.50	112.72
2	F	73	LEU	CA-CB-CG	5.71	136.28	116.30
2	F	40	SER	CA-CB-OG	-5.69	99.72	111.10
1	C	66	LYS	CG-CD-CE	-5.68	98.22	111.30
1	C	40	GLY	N-CA-C	-5.68	107.93	114.69
2	D	23	ASN	CA-C-N	5.68	128.14	120.65
2	D	23	ASN	C-N-CA	5.68	128.14	120.65
2	D	127	GLN	N-CA-C	5.67	118.41	109.96
2	B	221	VAL	CB-CA-C	5.67	119.20	110.82
2	F	32	TYR	O-C-N	-5.66	117.85	123.46
1	A	33	TYR	N-CA-C	5.66	118.00	109.23
1	G	48	TYR	CA-C-O	-5.66	115.39	121.45
2	H	82	VAL	N-CA-C	5.66	115.43	108.53
1	A	78	ILE	N-CA-C	5.66	116.43	108.17
2	B	28	TYR	CB-CA-C	-5.66	100.75	109.29
2	D	22	GLY	O-C-N	5.66	128.02	122.19
1	G	66	LYS	CG-CD-CE	-5.65	98.30	111.30
1	C	88	SER	CA-C-O	-5.64	115.07	120.94
2	H	113	ILE	CB-CA-C	-5.64	103.17	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	11	LEU	CB-CA-C	-5.64	99.78	109.65
1	G	44	ARG	CB-CA-C	5.64	119.69	109.37
1	G	44	ARG	N-CA-C	5.64	118.91	109.95
2	F	228	ILE	O-C-N	-5.63	117.27	123.18
1	C	80	GLU	N-CA-C	-5.62	104.54	111.40
2	D	89	TYR	N-CA-C	-5.62	100.77	109.14
1	A	50	TYR	CA-C-N	5.61	129.85	121.04
1	A	50	TYR	C-N-CA	5.61	129.85	121.04
1	C	115	SER	CB-CA-C	-5.59	102.18	110.62
1	G	66	LYS	CA-C-O	-5.58	115.26	121.51
1	E	7	SER	N-CA-C	-5.57	103.14	110.39
2	F	65	LYS	N-CA-C	-5.57	98.11	108.02
2	D	49	LEU	CA-C-N	5.57	130.09	123.19
2	D	49	LEU	C-N-CA	5.57	130.09	123.19
2	D	58	LEU	CA-C-N	-5.56	110.92	121.54
2	D	58	LEU	C-N-CA	-5.56	110.92	121.54
1	E	83	THR	CA-C-N	5.56	126.79	119.84
1	E	83	THR	C-N-CA	5.56	126.79	119.84
1	C	68	SER	N-CA-C	5.55	122.63	110.80
2	H	51	TYR	N-CA-C	-5.55	100.65	109.59
2	B	178	PRO	N-CA-C	5.55	121.05	113.84
2	B	224	LYS	CG-CD-CE	5.55	124.06	111.30
2	H	136	ASN	CB-CA-C	-5.53	104.74	111.82
1	G	63	GLY	CA-C-N	-5.53	113.25	122.21
1	G	63	GLY	C-N-CA	-5.53	113.25	122.21
2	H	27	LEU	N-CA-C	5.53	122.57	110.80
2	H	128	ASN	N-CA-C	5.52	118.92	110.20
2	D	5	ASP	N-CA-C	5.52	116.36	109.57
1	G	22	SER	N-CA-C	5.51	118.07	108.76
2	B	26	TYR	CA-C-O	-5.51	114.03	120.20
1	C	3	ALA	N-CA-C	-5.50	106.35	112.57
1	A	23	CYS	CA-C-N	5.50	131.64	122.73
1	A	23	CYS	C-N-CA	5.50	131.64	122.73
1	A	33	TYR	N-CA-CB	-5.50	101.30	111.53
2	H	98	LYS	N-CA-C	-5.49	99.10	110.80
1	E	80	GLU	CB-CA-C	5.49	121.34	110.42
2	H	212	LEU	CA-C-O	5.48	126.26	119.79
1	A	56	GLU	N-CA-CB	-5.47	102.02	111.55
1	E	73	GLU	CA-C-N	-5.47	113.13	122.33
1	E	73	GLU	C-N-CA	-5.47	113.13	122.33
1	G	34	TRP	N-CA-C	5.47	117.82	108.90
1	C	110	ALA	N-CA-C	5.47	119.95	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	30	ASN	CB-CA-C	-5.46	99.78	110.11
1	A	108	PHE	N-CA-C	5.46	122.43	110.80
2	B	224	LYS	CB-CG-CD	5.46	123.85	111.30
2	F	138	ARG	N-CA-C	5.46	119.12	109.96
1	G	66	LYS	CD-CE-NZ	-5.45	94.45	111.90
2	F	166	ILE	N-CA-C	-5.44	98.02	109.34
1	C	37	GLN	CA-C-N	-5.42	115.23	122.72
1	C	37	GLN	C-N-CA	-5.42	115.23	122.72
1	C	45	LEU	N-CA-C	-5.42	100.56	109.40
2	B	126	LEU	N-CA-C	-5.42	99.48	108.75
1	E	40	GLY	N-CA-C	-5.42	104.01	113.76
2	F	142	SER	O-C-N	-5.41	116.99	123.27
1	A	25	GLN	O-C-N	-5.41	116.16	123.19
2	F	26	TYR	N-CA-C	-5.41	105.55	111.82
2	B	98	LYS	N-CA-C	5.41	119.16	111.92
2	B	218	ASN	CA-C-O	-5.40	113.91	120.12
1	C	4	VAL	CB-CA-C	-5.40	102.44	111.29
2	F	3	GLN	CA-C-N	-5.40	115.02	120.31
2	F	3	GLN	C-N-CA	-5.40	115.02	120.31
1	G	52	ALA	CA-C-O	5.40	127.07	120.92
2	B	196	TYR	CB-CA-C	-5.39	100.21	109.65
1	C	50	TYR	N-CA-C	5.39	118.87	112.72
2	F	178	PRO	CA-C-N	5.39	129.79	122.19
2	F	178	PRO	C-N-CA	5.39	129.79	122.19
2	B	152	VAL	CA-C-N	5.38	128.51	120.87
2	B	152	VAL	C-N-CA	5.38	128.51	120.87
1	A	92	CYS	N-CA-C	-5.38	103.52	110.19
1	E	99	THR	N-CA-C	5.37	118.02	110.23
2	B	45	LEU	N-CA-C	-5.37	101.52	109.94
2	B	157	LEU	CB-CA-C	-5.37	99.44	110.38
2	F	201	ALA	CB-CA-C	5.36	117.16	109.11
2	D	47	HIS	N-CA-C	5.36	118.93	112.93
1	C	75	PHE	CA-C-O	-5.36	113.69	120.28
1	C	77	LEU	CA-C-O	-5.35	115.06	121.11
2	D	166	ILE	CB-CA-C	-5.35	105.03	112.04
1	E	66	LYS	N-CA-C	-5.35	102.07	110.36
2	D	68	LEU	CA-C-N	5.34	128.17	120.38
2	D	68	LEU	C-N-CA	5.34	128.17	120.38
1	C	99	THR	N-CA-C	5.34	117.97	110.23
2	F	49	LEU	CA-CB-CG	5.33	134.96	116.30
2	B	202	PRO	N-CA-C	5.33	120.57	111.68
2	B	198	MET	CB-CG-SD	5.32	128.66	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	LEU	CA-C-N	5.32	130.42	122.86
1	C	114	LEU	C-N-CA	5.32	130.42	122.86
1	G	59	ASP	N-CA-CB	5.32	119.48	110.49
1	E	4	VAL	CA-C-N	5.31	128.64	121.05
1	E	4	VAL	C-N-CA	5.31	128.64	121.05
2	D	107	THR	CA-CB-CG2	5.31	119.52	110.50
2	B	156	GLU	N-CA-C	5.30	117.47	111.11
1	C	112	THR	N-CA-C	-5.30	99.19	107.93
2	B	224	LYS	CA-CB-CG	5.29	124.69	114.10
1	G	6	GLN	N-CA-C	5.29	117.97	110.50
1	A	18	LYS	CG-CD-CE	-5.29	99.12	111.30
2	F	109	MET	O-C-N	5.29	129.55	122.73
2	H	127	GLN	CA-C-N	5.28	128.97	121.42
2	H	127	GLN	C-N-CA	5.28	128.97	121.42
2	B	64	VAL	CB-CA-C	5.28	118.83	110.81
2	H	91	VAL	N-CA-C	-5.27	100.03	107.98
2	F	117	GLU	N-CA-C	5.26	118.43	110.64
2	F	174	PHE	N-CA-C	5.26	116.70	111.07
2	B	46	ALA	N-CA-C	-5.25	106.03	112.90
2	B	108	CYS	N-CA-C	5.23	117.77	109.50
2	F	228	ILE	N-CA-CB	-5.22	104.15	111.25
1	C	25	GLN	N-CA-C	-5.21	101.27	109.50
2	D	214	MET	CB-CG-SD	-5.21	97.06	112.70
2	F	156	GLU	N-CA-C	-5.21	104.86	111.11
2	H	149	LYS	CA-C-N	5.21	131.49	121.54
2	H	149	LYS	C-N-CA	5.21	131.49	121.54
1	C	99	THR	CA-C-N	5.20	130.98	122.81
1	C	99	THR	C-N-CA	5.20	130.98	122.81
2	D	189	ASN	N-CA-C	5.20	121.88	110.80
2	B	84	VAL	N-CA-C	5.20	117.23	108.81
1	A	67	ALA	N-CA-C	5.19	116.87	109.14
2	F	43	LYS	CB-CG-CD	5.19	123.23	111.30
2	F	150	LYS	N-CA-C	5.19	119.51	112.04
2	D	26	TYR	CA-C-N	5.18	127.22	120.28
2	D	26	TYR	C-N-CA	5.18	127.22	120.28
2	H	175	ASN	N-CA-CB	5.18	119.25	110.49
2	F	66	THR	N-CA-C	-5.18	101.26	109.76
1	C	88	SER	N-CA-C	-5.18	100.79	107.73
2	F	46	ALA	N-CA-C	5.18	117.59	111.33
1	C	23	CYS	CA-CB-SG	5.15	126.25	114.40
1	G	63	GLY	O-C-N	5.15	129.17	122.42
2	D	125	ASN	N-CA-C	5.15	121.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	29	ASP	CB-CG-OD1	-5.14	106.57	118.40
1	A	8	PRO	CA-C-N	-5.13	113.38	122.26
1	A	8	PRO	C-N-CA	-5.13	113.38	122.26
1	G	33	TYR	CA-C-O	-5.13	114.76	120.66
2	F	182	GLY	N-CA-C	-5.13	101.03	113.18
1	C	38	ASP	CB-CA-C	5.12	118.20	109.75
2	D	160	LYS	CA-C-O	5.12	124.45	118.97
1	G	28	ASN	CA-C-O	-5.12	116.04	122.03
1	C	31	ASN	N-CA-C	5.11	117.44	110.24
1	A	27	ASN	N-CA-C	-5.11	105.36	111.03
2	F	187	ILE	N-CA-C	-5.11	98.72	109.34
2	F	60	ASN	N-CA-C	5.10	119.26	113.19
2	H	95	PHE	N-CA-C	5.10	121.66	110.80
2	F	66	THR	CA-CB-CG2	5.08	119.14	110.50
1	C	98	GLY	N-CA-C	5.08	118.39	112.50
1	E	6	GLN	N-CA-C	5.07	116.99	108.73
1	A	40	GLY	O-C-N	5.07	128.12	122.50
1	C	35	TYR	CA-C-N	-5.07	116.01	123.00
1	C	35	TYR	C-N-CA	-5.07	116.01	123.00
2	F	206	PHE	CB-CA-C	5.06	117.94	110.14
2	H	150	LYS	CA-C-N	5.06	129.56	121.66
2	H	150	LYS	C-N-CA	5.06	129.56	121.66
1	C	6	GLN	N-CA-C	5.06	118.27	107.70
2	D	88	ASN	N-CA-C	5.05	117.64	109.40
2	D	91	VAL	O-C-N	5.05	128.89	122.57
2	H	55	ASP	CB-CA-C	5.04	118.05	109.53
2	H	231	HIS	N-CA-C	5.04	118.37	107.49
1	G	29	HIS	CB-CA-C	-5.02	101.88	111.48
2	H	208	GLN	CA-C-O	-5.02	115.53	120.90
1	A	83	THR	CA-C-N	-5.01	113.87	119.19
1	A	83	THR	C-N-CA	-5.01	113.87	119.19
2	F	211	TYR	N-CA-C	-5.00	104.84	112.04

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ALA	Peptide
1	A	35	TYR	Peptide
1	A	54	SER	Mainchain
1	A	6	GLN	Peptide
1	A	61	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	75	PHE	Sidechain
2	B	125	ASN	Peptide
2	B	141	ILE	Peptide
2	B	22	GLY	Peptide
2	B	23	ASN	Peptide
2	B	27	LEU	Mainchain
2	D	34	SER	Peptide
1	E	93	ALA	Peptide
2	F	121	PHE	Peptide
2	F	235	LYS	Peptide
2	F	52	ASN	Peptide
2	F	74	ALA	Peptide
1	G	54	SER	Peptide
2	H	122	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	786	80	1
1	C	828	0	786	80	1
1	E	828	0	786	60	0
1	G	828	0	787	66	0
2	B	1904	0	1847	138	0
2	D	1913	0	1852	125	0
2	F	1906	0	1839	140	0
2	H	1922	0	1853	163	0
3	A	21	0	0	1	0
3	B	48	0	0	12	0
3	C	15	0	0	1	0
3	D	31	0	0	3	0
3	E	11	0	0	0	0
3	F	31	0	0	9	0
3	G	15	0	0	1	0
3	H	26	0	0	2	0
All	All	11155	0	10536	835	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 39.

All (835) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:CG2	1:A:26:THR:CB	1.76	1.60
1:E:80:GLU:CD	1:E:80:GLU:CG	1.75	1.55
2:B:27:LEU:CG	2:B:27:LEU:CD1	1.86	1.53
1:G:101:TYR:C	1:G:108:PHE:N	1.74	1.46
1:E:63:GLY:C	1:E:65:TYR:N	1.76	1.43
1:A:32:MET:SD	1:A:32:MET:CE	2.08	1.40
1:C:63:GLY:C	1:C:65:TYR:N	1.80	1.37
1:E:101:TYR:C	1:E:108:PHE:N	1.83	1.36
1:A:101:TYR:C	1:A:108:PHE:N	1.87	1.30
2:D:162:ARG:CG	2:D:162:ARG:HH11	1.47	1.23
1:A:87:THR:CG2	1:A:115:SER:HA	1.70	1.20
1:A:63:GLY:C	1:A:65:TYR:N	2.04	1.15
1:A:9:ARG:HH11	1:A:9:ARG:HB3	1.07	1.14
1:C:26:THR:O	1:C:27:ASN:HB2	1.35	1.14
2:D:56:LYS:HA	2:D:56:LYS:HE3	1.17	1.11
1:C:87:THR:HG23	1:C:115:SER:HA	1.32	1.10
2:D:13:LYS:HB3	2:D:180:GLU:OE1	1.49	1.10
2:D:162:ARG:HD3	2:D:198:MET:HE2	1.29	1.09
1:A:87:THR:HG23	1:A:115:SER:HA	1.12	1.07
2:D:162:ARG:HH11	2:D:162:ARG:HG3	0.96	1.07
1:C:83:THR:HG22	1:C:86:GLN:HG3	1.32	1.07
1:C:79:LEU:HD23	1:C:86:GLN:OE1	1.56	1.06
1:E:87:THR:HG23	1:E:114:LEU:O	1.58	1.03
1:A:87:THR:HG23	1:A:115:SER:CA	1.92	0.99
2:D:56:LYS:HE3	2:D:56:LYS:CA	1.92	0.98
2:D:162:ARG:HG3	2:D:162:ARG:NH1	1.64	0.98
2:B:190:ASN:C	2:B:190:ASN:HD22	1.70	0.98
1:C:14:VAL:O	1:C:17:GLU:HB2	1.64	0.97
2:F:195:TRP:O	2:F:196:TYR:HD2	1.44	0.96
2:H:155:GLN:HE21	2:H:215:TYR:HB3	1.25	0.96
1:A:39:THR:HG22	1:C:39:THR:O	1.65	0.96
1:E:4:VAL:HG12	1:E:4:VAL:O	1.66	0.94
1:A:24:GLN:OE1	1:A:74:GLN:NE2	1.99	0.94
1:E:32:MET:HE2	1:E:75:PHE:CB	1.97	0.94
2:F:37:LYS:HB2	2:F:116:HIS:CD2	2.03	0.93
2:D:127:GLN:NE2	2:D:224:LYS:HB3	1.84	0.93
1:G:87:THR:HG23	1:G:114:LEU:O	1.69	0.93
2:D:58:LEU:HD12	3:D:250:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:CE	1:E:75:PHE:HB3	1.98	0.93
2:F:35:ALA:HB3	2:F:84:VAL:CG2	1.99	0.92
1:G:18:LYS:NZ	1:G:18:LYS:HB3	1.83	0.92
1:G:11:LYS:HE3	1:G:19:VAL:HG13	1.51	0.92
1:E:28:ASN:OD1	1:E:72:GLN:NE2	2.03	0.92
1:C:7:SER:HB2	3:C:120:HOH:O	1.69	0.92
2:H:222:ASP:OD2	2:H:225:SER:HB3	1.68	0.91
2:F:52:ASN:HB3	3:F:245:HOH:O	1.70	0.91
2:B:138:ARG:HG3	2:B:138:ARG:HH11	1.35	0.91
2:H:56:LYS:H	2:H:57:LYS:HD3	1.35	0.91
2:H:103:THR:HG23	2:H:104:GLY:H	1.35	0.91
1:G:101:TYR:O	1:G:108:PHE:N	2.04	0.90
1:A:3:ALA:HA	1:A:26:THR:HG23	1.51	0.90
1:A:66:LYS:HG2	2:B:174:PHE:CG	2.08	0.89
2:H:39:LYS:HD3	2:H:79:ASP:HA	1.54	0.89
1:E:32:MET:HE1	1:E:75:PHE:HB3	1.54	0.89
2:F:206:PHE:HA	3:F:240:HOH:O	1.71	0.89
2:F:216:ASN:HD22	2:F:217:ASP:H	1.15	0.88
2:D:158:ASP:OD1	2:D:162:ARG:NH1	2.05	0.88
1:C:37:GLN:HG3	1:C:37:GLN:O	1.72	0.88
2:B:33:VAL:HG12	2:B:34:SER:H	1.38	0.87
1:C:101:TYR:O	1:C:108:PHE:CA	2.22	0.87
1:A:9:ARG:HB3	1:A:9:ARG:NH1	1.90	0.87
2:D:158:ASP:CG	2:D:162:ARG:HH12	1.81	0.87
1:C:26:THR:O	1:C:27:ASN:CB	2.20	0.86
1:G:17:GLU:HG3	1:G:18:LYS:N	1.90	0.86
2:D:60:ASN:O	2:D:61:TYR:HB3	1.74	0.85
2:H:55:ASP:OD1	2:H:57:LYS:HG2	1.77	0.85
2:F:49:LEU:HD11	2:F:78:LYS:HA	1.59	0.85
2:F:45:LEU:HD13	2:F:47:HIS:HE1	1.43	0.84
2:D:24:MET:CE	2:D:28:TYR:HE1	1.91	0.84
1:C:88:SER:OG	1:C:89:VAL:N	2.05	0.84
2:F:195:TRP:O	2:F:196:TYR:CD2	2.29	0.84
2:H:171:LEU:HD21	2:H:198:MET:HE2	1.60	0.83
2:F:222:ASP:OD2	2:F:225:SER:OG	1.94	0.83
2:D:136:ASN:O	2:D:137:LYS:HB2	1.79	0.82
2:F:35:ALA:HB3	2:F:84:VAL:HG23	1.62	0.82
1:E:32:MET:CE	1:E:75:PHE:CB	2.55	0.82
2:B:138:ARG:HH11	2:B:138:ARG:CG	1.91	0.82
1:A:31:ASN:ND2	1:A:50:TYR:HD1	1.77	0.81
1:C:101:TYR:O	1:C:108:PHE:HA	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LEU:CD1	3:D:250:HOH:O	2.25	0.81
2:F:216:ASN:HD22	2:F:217:ASP:N	1.78	0.81
1:G:87:THR:CG2	1:G:114:LEU:O	2.29	0.81
2:H:130:LEU:O	2:H:227:LYS:NZ	2.11	0.81
2:B:189:ASN:HD22	2:B:190:ASN:N	1.78	0.80
2:H:130:LEU:HD12	2:H:143:PHE:O	1.81	0.80
2:D:162:ARG:HD3	2:D:198:MET:CE	2.11	0.80
2:F:82:VAL:HG12	2:F:114:THR:O	1.81	0.80
2:D:162:ARG:O	2:D:166:ILE:HG13	1.82	0.80
1:E:44:ARG:HG3	1:E:44:ARG:HH21	1.47	0.80
1:G:87:THR:HG23	1:G:115:SER:HA	1.62	0.79
1:C:108:PHE:CD1	1:C:108:PHE:N	2.49	0.79
1:C:108:PHE:N	1:C:108:PHE:HD1	1.80	0.79
2:H:194:PHE:O	2:H:194:PHE:CD1	2.35	0.79
1:A:101:TYR:O	1:A:108:PHE:N	2.15	0.79
1:E:63:GLY:CA	1:E:65:TYR:N	2.46	0.79
1:G:11:LYS:HE3	1:G:19:VAL:CG1	2.12	0.79
2:D:159:ILE:HG22	2:D:159:ILE:O	1.82	0.78
2:H:126:LEU:HD21	2:H:148:ASP:HB3	1.66	0.78
1:G:21:LEU:HD12	1:G:77:LEU:HD23	1.65	0.78
2:B:33:VAL:HG12	2:B:34:SER:N	1.97	0.78
2:H:122:ASP:OD2	2:H:123:ASN:HB2	1.84	0.78
2:D:162:ARG:CG	2:D:162:ARG:NH1	2.28	0.78
2:H:51:TYR:HB2	2:H:53:ILE:HD12	1.66	0.77
1:A:31:ASN:ND2	1:A:50:TYR:CD1	2.52	0.77
2:H:147:THR:HG21	2:H:152:VAL:HG21	1.67	0.77
1:A:9:ARG:HH11	1:A:9:ARG:CB	1.95	0.76
2:F:82:VAL:HG11	2:F:113:ILE:CG2	2.15	0.76
2:B:24:MET:HE1	2:B:28:TYR:HE1	1.50	0.75
2:D:143:PHE:HE2	2:D:145:VAL:CG1	1.99	0.75
1:E:32:MET:HE2	1:E:75:PHE:HB2	1.69	0.75
1:E:101:TYR:C	1:E:108:PHE:CA	2.61	0.74
2:B:224:LYS:HB3	3:B:279:HOH:O	1.86	0.74
2:B:190:ASN:O	2:B:190:ASN:ND2	2.21	0.74
2:D:234:THR:O	2:D:235:LYS:NZ	2.18	0.74
2:D:226:VAL:O	2:D:227:LYS:HD3	1.88	0.74
2:H:42:ASP:OD1	2:H:43:LYS:N	2.21	0.74
1:C:54:SER:O	1:C:55:THR:HG22	1.87	0.73
2:D:33:VAL:O	2:D:85:TYR:HA	1.88	0.73
2:H:86:GLY:HA2	2:H:155:GLN:OE1	1.86	0.73
1:C:87:THR:CG2	1:C:115:SER:HA	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ASP:OD1	2:D:60:ASN:HB2	1.87	0.73
1:E:24:GLN:HE22	1:E:74:GLN:CD	1.97	0.73
2:F:83:ASP:HB2	2:F:114:THR:OG1	1.88	0.73
2:B:209:SER:HB2	3:B:254:HOH:O	1.88	0.72
2:D:68:LEU:HD11	2:D:113:ILE:HD12	1.71	0.72
2:D:127:GLN:HE21	2:D:224:LYS:HB3	1.54	0.72
2:H:155:GLN:HG3	2:H:215:TYR:CG	2.25	0.72
2:B:13:LYS:HB3	2:B:180:GLU:OE1	1.88	0.71
2:D:56:LYS:HA	2:D:56:LYS:CE	2.09	0.71
2:H:152:VAL:HG11	2:H:157:LEU:HD11	1.72	0.71
2:F:8:PRO:O	2:F:13:LYS:NZ	2.24	0.71
2:F:19:GLY:HA3	3:F:238:HOH:O	1.90	0.71
1:A:113:ARG:NH2	1:C:84:PRO:HB3	2.06	0.71
1:A:83:THR:O	1:A:116:VAL:HG11	1.91	0.70
2:F:167:ASN:HB3	3:F:265:HOH:O	1.92	0.70
2:B:162:ARG:O	2:B:166:ILE:HG13	1.90	0.70
2:B:184:ILE:HG13	2:B:230:VAL:HG22	1.74	0.70
2:F:11:LEU:HD11	2:F:183:TYR:CD2	2.27	0.70
1:C:83:THR:HG23	1:C:85:SER:HB2	1.74	0.69
2:D:184:ILE:HG23	2:D:184:ILE:O	1.92	0.69
2:H:31:HIS:CE1	2:H:88:ASN:ND2	2.61	0.69
1:G:49:SER:HB2	1:G:54:SER:O	1.91	0.69
1:E:101:TYR:O	1:E:108:PHE:N	2.24	0.69
2:H:88:ASN:H	2:H:88:ASN:HD22	1.40	0.69
2:H:130:LEU:HD12	2:H:131:VAL:N	2.07	0.69
2:B:20:THR:O	2:B:23:ASN:HB2	1.93	0.69
2:B:223:SER:O	2:B:225:SER:N	2.26	0.69
2:B:171:LEU:HD21	2:B:198:MET:HE3	1.74	0.68
1:C:9:ARG:HB3	1:C:9:ARG:NH1	2.08	0.68
1:G:18:LYS:HB3	1:G:18:LYS:HZ3	1.56	0.68
1:G:66:LYS:HB3	2:H:174:PHE:CE2	2.28	0.68
1:C:101:TYR:C	1:C:108:PHE:N	2.52	0.68
2:F:237:GLY:OXT	1:G:113:ARG:HG2	1.93	0.68
1:G:35:TYR:HA	1:G:44:ARG:O	1.93	0.68
1:A:87:THR:HG23	1:A:116:VAL:N	2.09	0.68
1:G:66:LYS:HB3	2:H:174:PHE:CD2	2.29	0.68
2:D:49:LEU:HD21	2:D:78:LYS:HB2	1.76	0.68
1:C:54:SER:O	1:C:55:THR:CG2	2.41	0.68
2:H:49:LEU:HD21	2:H:78:LYS:HA	1.76	0.68
2:H:86:GLY:CA	2:H:155:GLN:OE1	2.41	0.68
2:D:112:GLY:HA2	2:D:153:THR:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:GLN:O	1:E:74:GLN:HG3	1.88	0.67
1:G:14:VAL:O	1:G:15:THR:C	2.35	0.67
2:H:140:THR:C	2:H:141:ILE:HG23	2.19	0.67
1:G:12:VAL:HG11	1:G:117:LEU:HD11	1.75	0.67
2:H:123:ASN:ND2	2:H:125:ASN:HB2	2.10	0.67
2:H:86:GLY:HA3	2:H:109:MET:HE3	1.77	0.67
2:F:27:LEU:HA	2:F:31:HIS:HD2	1.60	0.67
2:H:181:THR:HG23	2:H:233:THR:HB	1.76	0.67
1:G:57:LYS:NZ	2:H:18:THR:O	2.26	0.67
2:B:6:PRO:HD3	2:B:195:TRP:CE2	2.30	0.67
1:G:59:ASP:O	1:G:61:PRO:HD3	1.95	0.67
1:A:87:THR:HG23	1:A:116:VAL:H	1.60	0.66
2:H:155:GLN:NE2	2:H:215:TYR:HB3	2.07	0.66
2:D:213:MET:O	2:D:216:ASN:HB2	1.94	0.66
2:F:95:PHE:CE2	2:F:106:LYS:HD3	2.30	0.66
2:H:77:TYR:O	2:H:79:ASP:N	2.29	0.66
1:A:3:ALA:HA	1:A:26:THR:CG2	2.26	0.66
1:A:31:ASN:HD22	1:A:50:TYR:HD1	1.42	0.66
2:D:43:LYS:HD3	2:D:48:ASP:O	1.96	0.66
1:A:68:SER:O	1:A:70:PRO:HD3	1.95	0.65
2:B:24:MET:CE	2:B:28:TYR:HE1	2.10	0.65
1:C:101:TYR:O	1:C:108:PHE:N	2.29	0.65
1:G:25:GLN:NE2	1:G:29:HIS:O	2.26	0.65
2:H:103:THR:CG2	2:H:104:GLY:H	2.06	0.65
2:H:233:THR:HG22	2:H:233:THR:O	1.95	0.65
1:E:10:ASN:O	1:E:11:LYS:HB2	1.96	0.65
2:D:24:MET:CE	2:D:28:TYR:CE1	2.77	0.64
2:D:52:ASN:OD1	2:D:63:LYS:HE2	1.96	0.64
2:B:19:GLY:H	2:B:204:ASP:HA	1.60	0.64
2:H:130:LEU:HD12	2:H:131:VAL:H	1.62	0.64
2:H:130:LEU:CD1	2:H:143:PHE:O	2.45	0.64
1:A:4:VAL:CG2	1:A:94:SER:HB3	2.27	0.64
2:B:8:PRO:O	2:B:13:LYS:HE3	1.98	0.64
2:B:103:THR:OG1	3:B:281:HOH:O	2.15	0.64
2:B:26:TYR:HE1	3:B:269:HOH:O	1.80	0.64
2:F:115:LYS:HD2	2:F:116:HIS:N	2.12	0.64
2:B:132:ARG:HD2	2:B:227:LYS:HE2	1.78	0.64
2:F:37:LYS:HB2	2:F:116:HIS:HD2	1.57	0.64
1:A:66:LYS:HE2	1:A:80:GLU:OE1	1.98	0.63
1:A:83:THR:O	1:A:116:VAL:CG1	2.46	0.63
2:D:47:HIS:HE1	2:D:67:GLU:OE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:HIS:ND1	2:F:116:HIS:C	2.56	0.63
1:E:44:ARG:HH21	1:E:44:ARG:CG	2.11	0.63
2:H:155:GLN:HE21	2:H:215:TYR:CB	2.05	0.63
2:B:171:LEU:HD21	2:B:198:MET:CE	2.28	0.63
2:B:190:ASN:C	2:B:190:ASN:ND2	2.42	0.63
2:D:95:PHE:CZ	2:D:106:LYS:HB2	2.34	0.63
2:F:95:PHE:CZ	2:F:106:LYS:HD3	2.34	0.63
2:H:147:THR:HG21	2:H:152:VAL:CG2	2.28	0.63
2:D:121:PHE:CE1	2:D:127:GLN:HB2	2.34	0.63
1:C:25:GLN:CG	1:C:25:GLN:O	2.46	0.63
2:F:45:LEU:HD13	2:F:47:HIS:CE1	2.31	0.63
2:H:80:GLU:HB3	2:H:82:VAL:HG13	1.80	0.63
2:D:3:GLN:HG3	2:D:194:PHE:HA	1.81	0.62
2:D:139:ASN:ND2	2:D:139:ASN:O	2.31	0.62
1:A:63:GLY:O	1:A:65:TYR:N	2.31	0.62
2:D:24:MET:HE2	2:D:28:TYR:CE1	2.34	0.62
2:B:87:SER:O	2:B:212:LEU:HD22	1.99	0.62
2:D:5:ASP:OD1	2:D:185:LYS:HE3	1.98	0.62
2:F:31:HIS:O	2:F:32:TYR:HB3	1.98	0.62
1:C:101:TYR:C	1:C:108:PHE:HA	2.25	0.62
1:E:63:GLY:C	1:E:65:TYR:CA	2.70	0.62
2:H:222:ASP:O	2:H:226:VAL:HG12	1.98	0.62
1:A:25:GLN:OE1	1:A:29:HIS:N	2.27	0.62
2:B:26:TYR:HH	2:B:90:TYR:HE1	1.47	0.62
2:D:66:THR:HA	2:D:109:MET:O	1.99	0.62
2:F:27:LEU:HA	2:F:31:HIS:CD2	2.35	0.62
1:G:66:LYS:HE3	1:G:80:GLU:HG2	1.82	0.62
2:B:52:ASN:OD1	2:B:63:LYS:HD3	1.99	0.62
2:B:107:THR:OG1	2:B:108:CYS:N	2.24	0.62
1:C:41:HIS:O	1:C:42:GLY:C	2.40	0.62
2:H:77:TYR:C	2:H:79:ASP:H	2.08	0.62
1:A:87:THR:HG22	1:A:115:SER:HA	1.77	0.62
2:B:101:LYS:C	2:B:103:THR:H	2.08	0.62
2:H:95:PHE:CZ	2:H:106:LYS:HG2	2.35	0.62
1:A:66:LYS:HG2	2:B:174:PHE:CD2	2.34	0.61
2:F:110:TYR:CD1	2:F:213:MET:HA	2.36	0.61
2:B:123:ASN:HB2	3:B:245:HOH:O	2.00	0.61
2:F:82:VAL:HG12	2:F:114:THR:C	2.25	0.61
2:H:194:PHE:O	2:H:194:PHE:HD1	1.81	0.61
1:A:23:CYS:SG	1:A:32:MET:HE1	2.41	0.61
2:B:25:LYS:HG2	3:B:271:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:HB3	3:B:268:HOH:O	2.00	0.61
1:E:44:ARG:HB2	1:E:60:ILE:CD1	2.30	0.61
2:F:80:GLU:OE2	2:F:80:GLU:HA	2.00	0.61
1:E:14:VAL:O	1:E:16:GLY:N	2.34	0.61
2:H:222:ASP:O	2:H:226:VAL:CG1	2.49	0.61
2:F:37:LYS:O	2:F:37:LYS:HG2	2.01	0.61
2:B:13:LYS:HD3	2:B:181:THR:HG22	1.81	0.61
2:B:26:TYR:OH	2:B:90:TYR:HE1	1.84	0.61
2:B:69:LEU:CD1	2:B:217:ASP:HA	2.31	0.61
2:B:217:ASP:OD1	2:B:218:ASN:N	2.33	0.61
2:F:55:ASP:HB3	2:F:58:LEU:O	2.01	0.61
1:G:87:THR:CG2	1:G:115:SER:HA	2.30	0.61
2:B:170:ASN:ND2	2:B:173:GLU:OE2	2.31	0.61
2:D:133:VAL:O	2:D:139:ASN:HA	2.01	0.61
1:G:11:LYS:CE	1:G:19:VAL:HG13	2.28	0.60
1:E:10:ASN:O	1:E:11:LYS:CB	2.49	0.60
2:B:24:MET:CE	2:B:28:TYR:CE1	2.84	0.60
2:F:35:ALA:CB	2:F:84:VAL:HG23	2.31	0.60
2:H:27:LEU:N	2:H:27:LEU:HD23	2.15	0.60
1:C:37:GLN:O	1:C:37:GLN:CG	2.46	0.60
2:F:11:LEU:HD11	2:F:183:TYR:HD2	1.65	0.60
1:G:24:GLN:OE1	1:G:74:GLN:HB2	2.01	0.60
2:H:103:THR:HG23	2:H:104:GLY:N	2.12	0.60
1:G:3:ALA:O	1:G:4:VAL:HG23	2.00	0.60
2:F:53:ILE:CD1	2:F:84:VAL:HG21	2.32	0.60
2:F:60:ASN:O	2:F:61:TYR:HB3	2.02	0.60
1:C:101:TYR:O	1:C:108:PHE:C	2.44	0.60
2:F:182:GLY:HA2	2:F:231:HIS:O	2.02	0.60
1:A:27:ASN:CB	1:A:29:HIS:CE1	2.85	0.60
1:C:74:GLN:NE2	1:C:76:SER:HB3	2.17	0.59
2:H:185:LYS:HE3	2:H:193:THR:HG21	1.84	0.59
1:A:69:ARG:HD2	1:A:74:GLN:O	2.02	0.59
1:C:51:GLY:HA3	2:D:91:VAL:HG22	1.84	0.59
2:H:88:ASN:HD22	2:H:88:ASN:N	2.00	0.59
2:F:136:ASN:OD1	2:F:233:THR:HA	2.03	0.59
2:H:40:SER:CB	2:H:49:LEU:HD22	2.32	0.59
1:A:52:ALA:HA	1:A:69:ARG:HG2	1.84	0.59
1:E:101:TYR:O	1:E:108:PHE:HA	2.03	0.59
2:B:138:ARG:CG	2:B:138:ARG:NH1	2.57	0.59
1:A:9:ARG:NH2	1:A:111:GLY:O	2.35	0.58
2:B:217:ASP:OD1	2:B:217:ASP:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:SER:C	2:D:16:GLU:H	2.10	0.58
2:H:39:LYS:CG	2:H:80:GLU:O	2.50	0.58
2:B:170:ASN:O	2:B:171:LEU:C	2.45	0.58
2:H:45:LEU:HD23	2:H:47:HIS:CE1	2.38	0.58
1:A:27:ASN:HB3	1:A:29:HIS:CE1	2.37	0.58
1:A:32:MET:CE	1:A:32:MET:CG	2.82	0.58
2:B:155:GLN:NE2	2:B:215:TYR:HB3	2.18	0.58
2:D:6:PRO:HG3	2:D:195:TRP:CE2	2.39	0.58
2:F:216:ASN:ND2	2:F:217:ASP:N	2.51	0.58
2:H:6:PRO:HD3	2:H:195:TRP:CE2	2.39	0.58
2:B:31:HIS:CE1	2:B:88:ASN:ND2	2.72	0.58
1:C:83:THR:HG23	1:C:85:SER:CB	2.33	0.58
2:F:166:ILE:O	2:F:170:ASN:HA	2.02	0.58
2:H:207:ASP:OD2	2:H:210:LYS:HB2	2.04	0.58
1:C:84:PRO:O	1:C:87:THR:OG1	2.06	0.58
2:B:187:ILE:HD13	2:B:227:LYS:HG2	1.85	0.58
2:F:81:VAL:O	2:F:115:LYS:HD3	2.04	0.57
1:A:24:GLN:HA	1:A:73:GLU:O	2.04	0.57
2:D:20:THR:O	2:D:23:ASN:HB2	2.03	0.57
2:D:27:LEU:HD21	2:D:208:GLN:HG2	1.86	0.57
2:H:39:LYS:HG3	2:H:80:GLU:O	2.04	0.57
2:D:143:PHE:CE2	2:D:145:VAL:HG13	2.39	0.57
1:G:66:LYS:HE3	1:G:80:GLU:CG	2.34	0.57
1:C:36:ARG:O	1:C:36:ARG:HG3	2.04	0.57
1:E:87:THR:CG2	1:E:114:LEU:O	2.45	0.57
2:H:31:HIS:CE1	2:H:88:ASN:HD21	2.21	0.57
2:B:27:LEU:HD22	2:B:212:LEU:HD11	1.86	0.57
2:F:34:SER:HA	2:F:84:VAL:O	2.03	0.57
2:F:110:TYR:HE1	2:F:209:SER:O	1.86	0.57
2:H:171:LEU:HD21	2:H:198:MET:CE	2.33	0.57
2:F:187:ILE:HG23	2:F:193:THR:HG22	1.87	0.57
2:D:15:SER:HB3	2:D:180:GLU:OE2	2.05	0.57
1:G:22:SER:HB3	1:G:74:GLN:OE1	2.05	0.57
2:F:187:ILE:HG23	2:F:193:THR:CG2	2.35	0.57
2:H:62:ASP:O	2:H:63:LYS:HG2	2.04	0.57
1:E:44:ARG:HB3	1:E:60:ILE:HD13	1.87	0.56
1:E:87:THR:HG23	1:E:115:SER:HA	1.87	0.56
2:F:58:LEU:HD13	2:F:60:ASN:ND2	2.20	0.56
2:D:68:LEU:N	2:D:68:LEU:HD22	2.20	0.56
1:E:14:VAL:O	1:E:15:THR:C	2.47	0.56
2:D:54:SER:O	2:D:55:ASP:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ASP:HA	2:D:61:TYR:CE2	2.40	0.56
2:H:155:GLN:HG3	2:H:215:TYR:CD1	2.40	0.56
2:D:56:LYS:CA	2:D:56:LYS:CE	2.74	0.56
2:F:81:VAL:HG12	2:F:116:HIS:HB3	1.87	0.56
1:G:37:GLN:O	1:G:37:GLN:HG2	2.03	0.56
2:H:126:LEU:CD2	2:H:148:ASP:HB3	2.34	0.56
2:B:156:GLU:O	2:B:160:LYS:HG3	2.06	0.56
2:B:200:PRO:O	2:B:201:ALA:C	2.47	0.56
1:G:9:ARG:O	1:G:9:ARG:HD3	2.05	0.56
2:H:225:SER:OG	2:H:226:VAL:N	2.33	0.56
1:A:70:PRO:HD2	1:A:74:GLN:HB3	1.88	0.56
2:B:27:LEU:CD1	2:B:27:LEU:CB	2.73	0.56
1:E:31:ASN:O	1:E:32:MET:HG2	2.06	0.56
2:F:35:ALA:HB3	2:F:84:VAL:HG22	1.83	0.56
2:F:71:GLU:O	2:F:71:GLU:HG2	2.06	0.56
1:G:15:THR:OG1	1:G:84:PRO:HD3	2.05	0.56
2:B:153:THR:HA	2:B:220:THR:HA	1.88	0.56
2:D:143:PHE:CE2	2:D:145:VAL:CG1	2.86	0.56
2:B:29:ASP:O	2:B:30:ASP:C	2.47	0.56
2:F:34:SER:HB2	2:F:85:TYR:CD1	2.40	0.56
2:D:152:VAL:HG11	2:D:157:LEU:HD21	1.87	0.56
1:A:41:HIS:C	1:A:42:GLY:O	2.49	0.55
1:A:37:GLN:O	1:A:38:ASP:OD2	2.24	0.55
2:B:189:ASN:HD22	2:B:190:ASN:H	1.51	0.55
1:C:9:ARG:NH1	1:C:9:ARG:CB	2.69	0.55
1:G:72:GLN:OE1	1:G:72:GLN:HA	2.06	0.55
2:D:118:GLY:O	2:D:150:LYS:HE3	2.05	0.55
2:F:201:ALA:HB1	2:F:202:PRO:HD2	1.88	0.55
2:H:48:ASP:HB3	2:H:67:GLU:HA	1.87	0.55
2:D:42:ASP:CG	2:D:43:LYS:H	2.14	0.55
1:E:44:ARG:CB	1:E:60:ILE:HD13	2.37	0.55
2:B:132:ARG:HD2	2:B:227:LYS:CE	2.37	0.55
2:F:194:PHE:H	2:F:194:PHE:HD2	1.53	0.55
2:H:171:LEU:O	2:H:177:SER:OG	2.21	0.55
2:B:219:LYS:HD2	2:B:220:THR:H	1.72	0.55
2:H:189:ASN:HD22	2:H:190:ASN:N	2.05	0.55
2:D:141:ILE:HG13	2:D:142:SER:N	2.22	0.55
2:D:188:GLU:HG2	3:D:238:HOH:O	2.06	0.55
2:D:228:ILE:HG22	2:D:229:GLU:N	2.22	0.55
2:H:149:LYS:O	2:H:223:SER:OG	2.24	0.55
1:E:108:PHE:N	1:E:108:PHE:CD1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:GLU:CG	1:G:18:LYS:N	2.66	0.55
2:H:123:ASN:HB3	2:H:125:ASN:H	1.72	0.55
2:D:6:PRO:HG3	2:D:195:TRP:CZ2	2.42	0.55
2:D:13:LYS:CB	2:D:180:GLU:OE1	2.38	0.55
2:H:89:TYR:CZ	2:H:209:SER:HB2	2.41	0.55
2:H:40:SER:HB2	2:H:49:LEU:HB3	1.89	0.55
1:A:66:LYS:HG2	2:B:174:PHE:CD1	2.42	0.54
1:E:38:ASP:OD1	1:E:88:SER:OG	2.20	0.54
1:E:28:ASN:O	1:E:28:ASN:CG	2.50	0.54
2:F:197:ASP:OD1	2:F:198:MET:N	2.39	0.54
2:B:7:MET:O	2:B:9:ASP:N	2.41	0.54
2:B:88:ASN:HD22	2:B:88:ASN:H	1.54	0.54
2:F:44:PHE:HD2	2:F:96:SER:HG	1.50	0.54
2:F:236:ASN:N	2:F:236:ASN:HD22	2.05	0.54
2:H:61:TYR:CG	2:H:107:THR:HG22	2.42	0.54
1:A:38:ASP:O	1:A:39:THR:C	2.50	0.54
1:C:74:GLN:HG3	1:C:75:PHE:N	2.06	0.54
1:A:38:ASP:OD1	1:A:44:ARG:NH1	2.40	0.54
1:A:88:SER:OG	1:A:89:VAL:N	2.40	0.54
2:B:184:ILE:O	2:B:184:ILE:HG23	2.07	0.54
1:C:68:SER:O	1:C:70:PRO:HD3	2.07	0.54
1:C:74:GLN:HE21	1:C:76:SER:HB3	1.71	0.54
2:D:24:MET:HE2	2:D:28:TYR:HE1	1.67	0.54
2:F:53:ILE:HD11	2:F:84:VAL:HG21	1.87	0.54
2:H:155:GLN:HG3	2:H:215:TYR:CD2	2.42	0.54
2:B:95:PHE:CZ	2:B:106:LYS:HG2	2.43	0.54
1:E:44:ARG:CB	1:E:60:ILE:CD1	2.86	0.54
2:F:186:PHE:C	2:F:187:ILE:HG13	2.32	0.54
2:H:102:VAL:HG12	2:H:102:VAL:O	2.07	0.54
2:H:151:SER:HA	2:H:221:VAL:O	2.08	0.54
1:E:79:LEU:O	1:E:80:GLU:C	2.51	0.54
2:B:47:HIS:NE2	2:B:67:GLU:OE1	2.32	0.54
1:C:9:ARG:HB3	1:C:9:ARG:CZ	2.37	0.54
2:F:120:HIS:O	2:F:150:LYS:NZ	2.41	0.54
2:H:129:VAL:HG12	2:H:130:LEU:N	2.22	0.54
1:E:32:MET:C	1:E:33:TYR:CD1	2.86	0.53
2:H:99:ASP:HB3	2:H:102:VAL:HA	1.89	0.53
1:A:45:LEU:HD21	1:A:48:TYR:CD1	2.43	0.53
1:A:57:LYS:HB3	1:A:61:PRO:HG3	1.91	0.53
2:F:19:GLY:CA	3:F:238:HOH:O	2.54	0.53
1:A:4:VAL:HG21	1:A:94:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TYR:C	1:C:108:PHE:CA	2.82	0.53
2:H:147:THR:CG2	2:H:152:VAL:HG21	2.39	0.53
2:H:194:PHE:CD1	2:H:194:PHE:C	2.86	0.53
1:E:32:MET:HE2	1:E:75:PHE:CG	2.43	0.53
2:H:140:THR:O	2:H:141:ILE:CG2	2.57	0.53
1:E:33:TYR:CD1	1:E:33:TYR:N	2.76	0.53
1:C:24:GLN:N	1:C:24:GLN:CD	2.67	0.53
2:D:76:LYS:HE2	2:D:77:TYR:CZ	2.44	0.53
2:B:123:ASN:CB	3:B:245:HOH:O	2.55	0.53
2:F:164:PHE:O	2:F:168:LYS:HD3	2.08	0.53
1:G:17:GLU:HG3	1:G:18:LYS:H	1.70	0.53
1:G:14:VAL:O	1:G:17:GLU:HB3	2.08	0.52
2:H:61:TYR:CG	2:H:107:THR:CG2	2.92	0.52
2:B:55:ASP:OD2	2:B:56:LYS:N	2.43	0.52
2:B:71:GLU:O	2:B:71:GLU:HG2	2.08	0.52
2:F:130:LEU:HD12	2:F:143:PHE:O	2.10	0.52
2:H:35:ALA:HB2	2:H:53:ILE:HG12	1.90	0.52
2:H:140:THR:O	2:H:141:ILE:HG23	2.09	0.52
2:F:180:GLU:HA	2:F:180:GLU:OE1	2.08	0.52
1:A:87:THR:HG23	1:A:115:SER:C	2.35	0.52
2:B:24:MET:O	2:B:25:LYS:C	2.52	0.52
2:F:45:LEU:CD1	2:F:47:HIS:HE1	2.16	0.52
2:F:62:ASP:HB2	3:F:261:HOH:O	2.09	0.52
2:H:162:ARG:O	2:H:166:ILE:HG13	2.10	0.52
1:C:9:ARG:HH11	1:C:9:ARG:CG	2.22	0.52
2:F:149:LYS:HE2	2:F:156:GLU:OE2	2.09	0.52
1:G:80:GLU:O	1:G:81:SER:CB	2.55	0.52
2:H:13:LYS:HD3	2:H:180:GLU:OE1	2.10	0.52
2:D:76:LYS:O	2:D:76:LYS:CG	2.56	0.52
2:D:194:PHE:HZ	2:D:221:VAL:HG11	1.74	0.52
2:B:33:VAL:CG1	2:B:34:SER:H	2.16	0.52
2:B:152:VAL:O	2:B:152:VAL:HG13	2.09	0.52
2:D:86:GLY:HA3	2:D:109:MET:HE3	1.92	0.52
2:F:157:LEU:HD12	2:F:186:PHE:HE2	1.75	0.52
2:H:184:ILE:HG13	2:H:230:VAL:HG22	1.92	0.52
2:F:152:VAL:HG11	2:F:157:LEU:HD21	1.91	0.52
2:B:39:LYS:HD2	2:B:79:ASP:O	2.10	0.52
1:C:69:ARG:HH21	1:C:69:ARG:CG	2.23	0.52
1:E:101:TYR:O	1:E:108:PHE:CA	2.58	0.52
1:G:4:VAL:HG12	1:G:109:GLY:CA	2.40	0.52
1:G:66:LYS:CB	2:H:174:PHE:CE2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:CG2	1:A:116:VAL:H	2.23	0.52
1:E:32:MET:CE	1:E:75:PHE:HB2	2.35	0.52
2:D:20:THR:HG21	2:D:174:PHE:CZ	2.46	0.51
2:D:47:HIS:H	2:D:47:HIS:CD2	2.28	0.51
2:D:121:PHE:CZ	2:D:127:GLN:HB2	2.45	0.51
2:D:159:ILE:O	2:D:159:ILE:CG2	2.54	0.51
2:H:214:MET:HE3	2:H:215:TYR:CE2	2.45	0.51
2:B:224:LYS:O	2:B:225:SER:HB3	2.11	0.51
2:D:136:ASN:HD21	2:D:234:THR:H	1.58	0.51
2:D:155:GLN:O	2:D:156:GLU:C	2.53	0.51
2:B:169:LYS:HB3	2:B:179:TYR:OH	2.09	0.51
2:D:76:LYS:O	2:D:76:LYS:HG3	2.09	0.51
1:G:83:THR:C	1:G:116:VAL:HG11	2.36	0.51
1:A:38:ASP:O	1:A:41:HIS:HB2	2.09	0.51
1:G:44:ARG:HB3	1:G:44:ARG:HH21	1.74	0.51
1:G:45:LEU:O	1:G:59:ASP:N	2.43	0.51
1:C:41:HIS:O	1:C:43:LEU:N	2.44	0.51
2:F:69:LEU:H	2:F:73:LEU:HD23	1.76	0.51
2:B:213:MET:O	2:B:216:ASN:HB2	2.11	0.51
2:D:143:PHE:HE2	2:D:145:VAL:HG12	1.74	0.51
2:F:11:LEU:CD1	2:F:183:TYR:HD2	2.22	0.51
1:C:25:GLN:OE1	1:C:29:HIS:N	2.41	0.51
2:F:90:TYR:O	2:F:92:ASN:N	2.44	0.51
1:G:31:ASN:N	1:G:31:ASN:HD22	2.08	0.51
1:E:25:GLN:O	1:E:25:GLN:HG3	2.10	0.51
2:D:43:LYS:NZ	2:D:78:LYS:HD2	2.26	0.50
2:F:110:TYR:OH	2:F:209:SER:OG	2.29	0.50
2:F:193:THR:C	3:F:244:HOH:O	2.53	0.50
2:H:128:ASN:HD22	2:H:144:GLU:CD	2.19	0.50
2:B:33:VAL:CG1	2:B:34:SER:N	2.71	0.50
2:F:33:VAL:N	2:F:86:GLY:O	2.41	0.50
2:F:205:LYS:HD3	2:F:205:LYS:N	2.25	0.50
2:H:51:TYR:HB2	2:H:53:ILE:CD1	2.39	0.50
2:F:166:ILE:HG22	2:F:167:ASN:N	2.26	0.50
1:A:114:LEU:HG	1:A:115:SER:N	2.27	0.50
1:C:25:GLN:OE1	1:C:29:HIS:HB2	2.11	0.50
1:C:33:TYR:CD1	1:C:33:TYR:N	2.79	0.50
2:F:7:MET:HB3	2:F:8:PRO:HD2	1.93	0.50
2:H:45:LEU:HD23	2:H:47:HIS:NE2	2.26	0.50
1:A:33:TYR:HB2	1:A:93:ALA:HB3	1.94	0.50
2:H:77:TYR:C	2:H:79:ASP:N	2.66	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLY:N	2:B:204:ASP:HA	2.26	0.50
2:D:162:ARG:CD	2:D:198:MET:HE2	2.22	0.50
1:E:87:THR:CG2	1:E:115:SER:HA	2.42	0.50
2:F:204:ASP:OD1	2:F:205:LYS:HE3	2.10	0.50
1:G:55:THR:HB	3:G:121:HOH:O	2.11	0.50
2:H:13:LYS:HB3	2:H:180:GLU:OE1	2.12	0.50
2:H:27:LEU:HA	2:H:31:HIS:HD2	1.75	0.50
2:H:212:LEU:O	2:H:213:MET:C	2.55	0.50
2:F:194:PHE:N	3:F:244:HOH:O	2.43	0.50
2:F:68:LEU:HD11	2:F:113:ILE:CD1	2.42	0.49
1:G:12:VAL:HG11	1:G:117:LEU:CD1	2.42	0.49
1:A:36:ARG:HG2	1:A:46:ILE:HD11	1.94	0.49
2:D:134:TYR:CE2	2:D:139:ASN:HB2	2.46	0.49
2:H:27:LEU:HA	2:H:31:HIS:CD2	2.48	0.49
1:C:38:ASP:OD1	1:C:88:SER:HB2	2.12	0.49
1:C:82:ALA:HB1	1:C:116:VAL:HG21	1.94	0.49
2:D:165:LEU:O	2:D:171:LEU:HB2	2.12	0.49
2:D:39:LYS:HE2	2:D:79:ASP:O	2.13	0.49
2:D:51:TYR:HB2	2:D:53:ILE:HD12	1.94	0.49
2:H:140:THR:C	2:H:141:ILE:CG2	2.85	0.49
2:D:162:ARG:HD2	2:D:172:TYR:CE1	2.47	0.49
2:H:2:SER:O	2:H:3:GLN:HB2	2.12	0.49
2:D:128:ASN:HD22	2:D:144:GLU:CD	2.21	0.49
1:E:14:VAL:H	1:E:17:GLU:HG2	1.77	0.49
1:E:44:ARG:HB2	1:E:60:ILE:HD12	1.93	0.49
1:G:51:GLY:HA3	2:H:91:VAL:HG22	1.94	0.49
2:H:39:LYS:HG2	2:H:80:GLU:O	2.13	0.49
1:A:113:ARG:HH22	1:C:84:PRO:HB3	1.78	0.49
1:C:9:ARG:CB	1:C:9:ARG:HH11	2.24	0.49
2:D:135:GLU:HA	2:D:232:LEU:O	2.13	0.49
2:F:110:TYR:HD1	2:F:212:LEU:C	2.21	0.49
2:F:204:ASP:C	2:F:205:LYS:HD3	2.37	0.49
2:B:6:PRO:HD3	2:B:195:TRP:CD2	2.47	0.49
2:H:186:PHE:O	2:H:193:THR:HA	2.12	0.49
1:A:9:ARG:NH1	1:A:9:ARG:CB	2.67	0.49
2:F:6:PRO:HG3	2:F:195:TRP:CE2	2.48	0.49
2:F:187:ILE:HA	2:F:193:THR:HG22	1.95	0.49
1:A:54:SER:HA	2:B:23:ASN:OD1	2.13	0.48
2:B:24:MET:HE2	2:B:28:TYR:CE1	2.48	0.48
2:B:69:LEU:HD12	2:B:217:ASP:HA	1.95	0.48
2:H:55:ASP:HB2	2:H:61:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:LYS:O	2:H:170:ASN:HB2	2.13	0.48
2:F:89:TYR:C	2:F:89:TYR:CD2	2.91	0.48
2:F:216:ASN:ND2	2:F:217:ASP:H	1.96	0.48
2:D:219:LYS:HE2	2:D:221:VAL:HG12	1.95	0.48
2:D:14:SER:C	2:D:16:GLU:N	2.70	0.48
2:D:102:VAL:HG23	2:D:102:VAL:O	2.14	0.48
2:F:165:LEU:O	2:F:166:ILE:O	2.31	0.48
2:F:110:TYR:CE1	2:F:209:SER:O	2.65	0.48
1:G:34:TRP:HD1	1:G:75:PHE:CE2	2.32	0.48
2:F:200:PRO:HB2	2:F:206:PHE:CD1	2.48	0.48
2:B:8:PRO:O	2:B:13:LYS:CE	2.62	0.48
2:B:27:LEU:CD1	2:B:27:LEU:CD2	2.88	0.48
2:D:94:TYR:O	2:D:95:PHE:HB3	2.12	0.48
2:F:119:ASN:O	2:F:150:LYS:HG3	2.13	0.48
1:G:77:LEU:HG	1:G:78:ILE:N	2.29	0.48
2:B:21:MET:O	2:B:24:MET:HB3	2.14	0.47
2:B:139:ASN:ND2	2:B:139:ASN:O	2.47	0.47
1:C:43:LEU:HA	1:C:43:LEU:HD12	1.56	0.47
1:C:67:ALA:O	1:C:68:SER:CB	2.60	0.47
2:H:7:MET:HE2	2:H:7:MET:HA	1.96	0.47
2:H:33:VAL:O	2:H:85:TYR:HA	2.13	0.47
2:B:188:GLU:HG3	2:B:192:ASN:HB3	1.96	0.47
2:F:82:VAL:HG11	2:F:113:ILE:HG23	1.96	0.47
1:A:23:CYS:HB2	1:A:34:TRP:CZ2	2.49	0.47
2:H:110:TYR:CE2	2:H:213:MET:HG3	2.50	0.47
2:B:12:HIS:HB2	2:B:197:ASP:OD2	2.15	0.47
1:G:18:LYS:NZ	1:G:18:LYS:CB	2.68	0.47
1:G:19:VAL:HG23	1:G:82:ALA:HB2	1.96	0.47
2:H:24:MET:O	2:H:27:LEU:HB2	2.15	0.47
1:A:26:THR:CG2	1:A:26:THR:CA	2.80	0.47
2:D:49:LEU:HD21	2:D:78:LYS:CB	2.42	0.47
2:F:45:LEU:CD1	2:F:47:HIS:CE1	2.95	0.47
2:F:195:TRP:C	2:F:196:TYR:CD2	2.92	0.47
1:G:21:LEU:O	1:G:76:SER:HB2	2.14	0.47
1:G:114:LEU:HD21	1:G:116:VAL:CG2	2.44	0.47
2:H:49:LEU:CD2	2:H:78:LYS:HA	2.44	0.47
2:B:213:MET:HE3	3:B:244:HOH:O	2.13	0.47
2:D:68:LEU:HD22	2:D:68:LEU:H	1.77	0.47
2:D:219:LYS:CE	2:D:220:THR:O	2.63	0.47
2:F:7:MET:CB	2:F:8:PRO:HD2	2.45	0.47
2:F:115:LYS:CD	2:F:116:HIS:N	2.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:TYR:HB3	2:B:233:THR:O	2.15	0.47
1:C:44:ARG:HE	1:C:44:ARG:HB2	1.58	0.47
2:H:37:LYS:HE2	2:H:116:HIS:CE1	2.50	0.47
2:H:184:ILE:O	2:H:195:TRP:HA	2.15	0.47
1:A:38:ASP:HB2	1:A:44:ARG:NH1	2.30	0.46
2:B:113:ILE:HD13	2:B:113:ILE:HG21	1.56	0.46
1:C:30:ASN:O	1:C:69:ARG:NH1	2.42	0.46
1:E:93:ALA:HB1	1:E:100:LEU:HD22	1.96	0.46
2:B:136:ASN:O	2:B:138:ARG:NH1	2.48	0.46
1:C:25:GLN:O	1:C:25:GLN:HG3	2.09	0.46
2:D:24:MET:HE1	2:D:28:TYR:HE1	1.76	0.46
2:H:227:LYS:HZ2	2:H:227:LYS:HA	1.79	0.46
2:B:13:LYS:CB	2:B:180:GLU:OE1	2.61	0.46
1:E:12:VAL:HA	1:E:115:SER:O	2.14	0.46
1:E:32:MET:HE2	1:E:75:PHE:CD2	2.51	0.46
2:F:188:GLU:HB2	2:F:192:ASN:HB3	1.96	0.46
1:C:32:MET:C	1:C:33:TYR:CD1	2.94	0.46
2:D:182:GLY:HA2	2:D:231:HIS:O	2.15	0.46
2:H:82:VAL:HG11	2:H:113:ILE:CG2	2.46	0.46
2:H:132:ARG:HG2	2:H:142:SER:HB3	1.96	0.46
2:H:218:ASN:HA	3:H:242:HOH:O	2.14	0.46
1:A:45:LEU:HD21	1:A:48:TYR:HD1	1.80	0.46
2:D:42:ASP:OD2	2:D:43:LYS:N	2.48	0.46
2:H:85:TYR:O	2:H:112:GLY:HA3	2.16	0.46
2:B:110:TYR:CD1	2:B:212:LEU:O	2.68	0.46
1:C:33:TYR:HB3	1:C:45:LEU:CD1	2.46	0.46
2:F:170:ASN:O	2:F:178:PRO:CD	2.64	0.46
2:H:6:PRO:HB2	2:H:11:LEU:HG	1.98	0.46
2:D:46:ALA:HB1	2:D:71:GLU:HB2	1.97	0.46
2:H:61:TYR:CD2	2:H:107:THR:HG21	2.51	0.46
2:D:12:HIS:O	2:D:181:THR:HG22	2.15	0.46
2:D:162:ARG:HD2	2:D:172:TYR:HE1	1.80	0.46
1:G:12:VAL:HA	1:G:115:SER:O	2.16	0.46
2:B:5:ASP:OD1	2:B:185:LYS:NZ	2.34	0.46
2:B:24:MET:HA	2:B:24:MET:HE3	1.97	0.46
1:G:87:THR:HG22	1:G:114:LEU:O	2.12	0.46
1:C:3:ALA:HA	1:C:26:THR:HB	1.98	0.46
2:D:31:HIS:CE1	2:D:88:ASN:ND2	2.84	0.46
1:E:46:ILE:HG22	1:E:47:HIS:CD2	2.51	0.46
2:F:41:VAL:O	2:F:42:ASP:CB	2.64	0.46
1:A:23:CYS:SG	1:A:32:MET:CE	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.77	0.45
2:B:100:GLY:O	2:B:102:VAL:N	2.49	0.45
1:C:65:TYR:CD1	1:C:77:LEU:HD11	2.51	0.45
2:H:99:ASP:HB3	2:H:102:VAL:CA	2.47	0.45
2:B:27:LEU:C	2:B:31:HIS:HD2	2.24	0.45
1:C:83:THR:HG22	1:C:86:GLN:CG	2.24	0.45
1:C:86:GLN:O	1:C:90:TYR:OH	2.28	0.45
2:D:43:LYS:HB2	2:D:43:LYS:HE2	1.49	0.45
2:H:21:MET:HE3	2:H:177:SER:HB2	1.98	0.45
2:B:31:HIS:HB2	3:B:241:HOH:O	2.17	0.45
2:D:126:LEU:HD22	2:D:147:THR:O	2.17	0.45
2:D:206:PHE:CE2	2:D:208:GLN:HG3	2.52	0.45
1:E:36:ARG:HG2	1:E:60:ILE:HD11	1.99	0.45
2:B:70:ASN:HB2	2:B:71:GLU:H	1.42	0.45
2:F:49:LEU:HD22	2:F:74:ALA:HB1	1.98	0.45
1:C:28:ASN:HA	1:C:72:GLN:HG2	1.99	0.45
1:A:46:ILE:CD1	1:A:77:LEU:HD21	2.46	0.45
1:E:11:LYS:HE3	1:E:19:VAL:HG13	1.99	0.45
1:E:71:SER:OG	1:E:74:GLN:HB3	2.17	0.45
2:F:155:GLN:O	2:F:156:GLU:C	2.59	0.45
2:F:165:LEU:O	2:F:166:ILE:C	2.55	0.45
2:F:206:PHE:HB2	3:F:240:HOH:O	2.17	0.45
2:H:55:ASP:HB2	2:H:61:TYR:CE2	2.51	0.45
2:H:56:LYS:C	2:H:57:LYS:HD2	2.41	0.45
2:H:67:GLU:HG2	2:H:110:TYR:CE2	2.52	0.45
2:H:69:LEU:HG	2:H:69:LEU:O	2.16	0.45
2:B:32:TYR:HD1	2:B:33:VAL:O	1.99	0.45
2:F:89:TYR:HD1	2:F:212:LEU:HD12	1.82	0.45
2:H:89:TYR:CE2	2:H:209:SER:HB2	2.51	0.45
1:A:46:ILE:HD12	1:A:77:LEU:HD21	1.99	0.45
2:B:175:ASN:C	2:B:175:ASN:ND2	2.74	0.45
2:H:218:ASN:O	2:H:219:LYS:C	2.59	0.45
2:F:81:VAL:HG12	2:F:116:HIS:CB	2.47	0.45
2:H:42:ASP:OD1	2:H:43:LYS:O	2.35	0.45
1:A:60:ILE:O	1:A:60:ILE:HG13	2.17	0.44
2:B:169:LYS:O	2:B:170:ASN:HB2	2.16	0.44
1:C:69:ARG:HD2	1:C:71:SER:O	2.17	0.44
2:F:90:TYR:CD1	2:F:90:TYR:N	2.85	0.44
1:G:38:ASP:O	1:G:39:THR:C	2.59	0.44
2:H:97:SER:HB3	2:H:98:LYS:H	1.46	0.44
2:B:27:LEU:HD23	2:B:27:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:CG2	1:C:85:SER:HB2	2.45	0.44
1:E:11:LYS:O	1:E:114:LEU:HD12	2.17	0.44
2:F:5:ASP:HA	2:F:6:PRO:HD3	1.79	0.44
1:A:23:CYS:CB	1:A:34:TRP:CZ2	3.01	0.44
2:D:219:LYS:HE2	2:D:220:THR:O	2.17	0.44
2:D:49:LEU:HA	2:D:49:LEU:HD23	1.55	0.44
1:C:77:LEU:HD12	1:C:78:ILE:H	1.83	0.44
1:E:44:ARG:HG3	1:E:44:ARG:NH2	2.25	0.44
2:H:67:GLU:O	2:H:67:GLU:HG3	2.18	0.44
2:B:31:HIS:HA	2:B:57:LYS:HE2	1.99	0.44
1:C:31:ASN:ND2	1:C:50:TYR:CD1	2.86	0.44
2:D:5:ASP:HA	2:D:6:PRO:HD3	1.75	0.44
2:F:20:THR:O	2:F:20:THR:HG22	2.18	0.44
2:F:55:ASP:OD2	2:F:60:ASN:HB2	2.17	0.44
2:H:99:ASP:HB3	2:H:102:VAL:N	2.32	0.44
2:H:166:ILE:HD11	2:H:172:TYR:CD1	2.52	0.44
2:H:236:ASN:ND2	2:H:236:ASN:N	2.66	0.44
2:B:18:THR:N	2:B:203:GLY:O	2.32	0.44
2:D:228:ILE:CG2	2:D:229:GLU:N	2.81	0.44
2:F:3:GLN:HE21	2:F:3:GLN:HB2	1.57	0.44
2:F:35:ALA:CB	2:F:84:VAL:CG2	2.85	0.44
2:F:53:ILE:HD13	2:F:84:VAL:HG21	1.99	0.44
2:F:184:ILE:HG23	2:F:184:ILE:O	2.16	0.44
2:H:150:LYS:O	2:H:223:SER:N	2.37	0.44
2:H:202:PRO:HG3	3:H:244:HOH:O	2.17	0.44
1:A:69:ARG:HH21	1:A:69:ARG:HD3	1.61	0.43
1:C:66:LYS:HZ3	1:C:66:LYS:HG3	1.48	0.43
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.79	0.43
2:H:207:ASP:HB3	2:H:210:LYS:HB3	2.00	0.43
2:B:65:LYS:HD3	2:B:95:PHE:HB3	2.01	0.43
2:B:170:ASN:HD22	2:B:173:GLU:CD	2.24	0.43
2:H:227:LYS:HZ2	2:H:228:ILE:H	1.66	0.43
1:C:63:GLY:CA	1:C:65:TYR:N	2.73	0.43
2:D:168:LYS:HB2	2:D:168:LYS:HE2	1.36	0.43
1:E:77:LEU:C	1:E:78:ILE:HG13	2.43	0.43
2:F:207:ASP:OD2	2:F:210:LYS:HB2	2.19	0.43
2:F:40:SER:CB	2:F:49:LEU:HD12	2.48	0.43
2:F:152:VAL:N	2:F:221:VAL:O	2.43	0.43
2:H:61:TYR:HA	2:H:105:GLY:HA3	1.99	0.43
2:H:236:ASN:N	2:H:236:ASN:HD22	2.16	0.43
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TYR:CD1	2:B:32:TYR:C	2.96	0.43
2:B:84:VAL:O	2:B:85:TYR:HB2	2.18	0.43
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.84	0.43
2:H:180:GLU:HG2	2:H:235:LYS:HB2	2.00	0.43
2:B:3:GLN:OE1	2:B:195:TRP:CD1	2.72	0.43
2:B:7:MET:C	2:B:9:ASP:H	2.25	0.43
2:B:26:TYR:C	2:B:28:TYR:H	2.25	0.43
2:F:6:PRO:HG3	2:F:195:TRP:CD2	2.54	0.43
2:F:87:SER:HB3	2:F:159:ILE:HD11	2.00	0.43
2:F:115:LYS:HE3	2:F:117:GLU:HB2	2.00	0.43
2:H:135:GLU:O	2:H:136:ASN:HB2	2.19	0.43
1:A:52:ALA:HA	1:A:69:ARG:CG	2.48	0.43
2:B:47:HIS:HB2	2:B:70:ASN:HA	2.01	0.43
2:B:136:ASN:HD21	2:B:234:THR:HG23	1.84	0.43
2:B:166:ILE:HG23	2:B:166:ILE:HD13	1.58	0.43
2:B:171:LEU:HD12	2:B:171:LEU:HA	1.42	0.43
1:C:83:THR:CG2	1:C:86:GLN:HG3	2.23	0.43
1:E:23:CYS:HB2	1:E:34:TRP:CZ2	2.53	0.43
2:F:162:ARG:NH1	2:F:172:TYR:OH	2.50	0.43
2:H:152:VAL:CG1	2:H:157:LEU:HD11	2.46	0.43
2:B:127:GLN:NE2	2:B:224:LYS:HA	2.34	0.43
2:B:134:TYR:CB	3:B:275:HOH:O	2.65	0.43
1:C:47:HIS:ND1	1:C:57:LYS:HA	2.33	0.43
1:E:63:GLY:N	1:E:65:TYR:N	2.66	0.43
1:G:4:VAL:HG12	1:G:109:GLY:HA3	2.00	0.43
2:H:152:VAL:HG13	2:H:152:VAL:O	2.17	0.43
2:H:181:THR:HG23	2:H:233:THR:CB	2.48	0.43
2:B:55:ASP:OD2	2:B:55:ASP:C	2.62	0.43
2:B:134:TYR:HB3	3:B:275:HOH:O	2.19	0.43
2:H:7:MET:HA	2:H:7:MET:CE	2.48	0.43
2:D:219:LYS:HE2	2:D:221:VAL:CG1	2.49	0.43
1:G:28:ASN:CG	1:G:28:ASN:O	2.56	0.43
1:G:54:SER:HA	2:H:23:ASN:OD1	2.19	0.43
2:H:155:GLN:NE2	2:H:215:TYR:CB	2.76	0.43
1:A:87:THR:CG2	1:A:115:SER:CA	2.63	0.42
2:F:128:ASN:HA	2:F:145:VAL:O	2.19	0.42
1:G:12:VAL:CG1	1:G:117:LEU:CD1	2.97	0.42
2:B:208:GLN:O	2:B:212:LEU:HD12	2.19	0.42
2:D:68:LEU:H	2:D:68:LEU:CD2	2.32	0.42
1:A:45:LEU:HD23	1:A:58:GLY:HA2	2.00	0.42
2:F:21:MET:HE3	2:F:177:SER:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:VAL:HG23	2:F:88:ASN:HB3	2.02	0.42
2:F:77:TYR:O	2:F:78:LYS:C	2.63	0.42
1:G:23:CYS:HB2	1:G:34:TRP:CZ2	2.54	0.42
1:G:32:MET:HA	1:G:94:SER:HA	2.00	0.42
1:G:83:THR:O	1:G:116:VAL:HG11	2.20	0.42
2:H:189:ASN:HD22	2:H:189:ASN:C	2.27	0.42
1:E:93:ALA:HA	1:E:101:TYR:O	2.19	0.42
2:F:127:GLN:O	2:F:146:GLN:HA	2.19	0.42
2:H:48:ASP:HB2	2:H:66:THR:O	2.19	0.42
1:A:9:ARG:HH22	1:A:111:GLY:N	2.17	0.42
2:D:27:LEU:HD11	2:D:208:GLN:HG2	2.01	0.42
2:H:45:LEU:CD2	2:H:47:HIS:CE1	3.03	0.42
1:A:44:ARG:HE	1:A:44:ARG:HB2	1.47	0.42
2:B:184:ILE:HG13	2:B:230:VAL:CG2	2.48	0.42
1:C:116:VAL:O	1:C:116:VAL:HG12	2.16	0.42
2:F:82:VAL:CG1	2:F:113:ILE:CG2	2.93	0.42
2:F:214:MET:HE3	2:F:215:TYR:CZ	2.55	0.42
1:G:55:THR:O	2:H:23:ASN:ND2	2.49	0.42
2:B:24:MET:HE2	2:B:28:TYR:CD1	2.55	0.42
2:D:2:SER:OG	2:D:192:ASN:OD1	2.23	0.42
2:F:89:TYR:CZ	2:F:209:SER:HB2	2.55	0.42
2:H:216:ASN:C	2:H:218:ASN:N	2.78	0.42
2:B:69:LEU:HD11	2:B:217:ASP:HA	2.02	0.42
2:D:162:ARG:CD	2:D:198:MET:CE	2.90	0.42
2:D:195:TRP:CD2	2:D:195:TRP:O	2.73	0.42
2:F:151:SER:HA	2:F:221:VAL:O	2.19	0.42
2:F:164:PHE:C	2:F:164:PHE:CD2	2.98	0.42
2:B:86:GLY:N	2:B:109:MET:HE1	2.34	0.42
1:C:36:ARG:O	1:C:36:ARG:CG	2.68	0.42
2:D:50:ILE:HG21	2:D:50:ILE:HD13	1.39	0.42
1:G:17:GLU:O	1:G:82:ALA:N	2.45	0.42
1:C:33:TYR:HB3	1:C:45:LEU:HD11	2.02	0.41
1:C:114:LEU:HG	1:C:115:SER:N	2.34	0.41
2:D:91:VAL:O	2:D:92:ASN:HB3	2.20	0.41
2:B:84:VAL:HG12	2:B:85:TYR:N	2.36	0.41
2:B:136:ASN:ND2	2:B:234:THR:HG23	2.34	0.41
2:D:94:TYR:O	2:D:94:TYR:CD2	2.74	0.41
2:D:181:THR:OG1	2:D:233:THR:OG1	2.38	0.41
2:F:187:ILE:HD11	2:F:229:GLU:CG	2.50	0.41
2:B:47:HIS:O	2:B:47:HIS:CD2	2.74	0.41
2:D:65:LYS:HE2	2:D:65:LYS:HB3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:LYS:HD2	2:F:79:ASP:C	2.45	0.41
2:F:194:PHE:CE2	2:F:219:LYS:HE3	2.55	0.41
2:H:62:ASP:C	2:H:63:LYS:CG	2.93	0.41
2:H:77:TYR:O	2:H:78:LYS:C	2.63	0.41
1:A:67:ALA:O	1:A:68:SER:HB2	2.20	0.41
2:D:190:ASN:OD1	2:D:190:ASN:C	2.64	0.41
2:B:171:LEU:O	2:B:177:SER:OG	2.36	0.41
2:H:38:VAL:O	2:H:82:VAL:HG22	2.21	0.41
2:H:54:SER:HB2	2:H:62:ASP:HB2	2.02	0.41
1:A:62:ASP:HB2	3:A:132:HOH:O	2.19	0.41
1:C:25:GLN:O	1:C:25:GLN:HG2	2.17	0.41
2:F:87:SER:O	2:F:212:LEU:HD13	2.21	0.41
1:G:2:ALA:O	1:G:3:ALA:HB3	2.20	0.41
2:H:13:LYS:HZ2	2:H:13:LYS:HG2	1.66	0.41
1:A:32:MET:HE2	1:A:32:MET:HB3	2.02	0.41
2:B:101:LYS:C	2:B:103:THR:N	2.73	0.41
1:C:31:ASN:HA	1:C:49:SER:O	2.20	0.41
1:C:99:THR:HG23	1:E:100:LEU:O	2.19	0.41
2:H:56:LYS:N	2:H:57:LYS:HD3	2.18	0.41
1:G:13:ALA:HB3	1:G:116:VAL:HG22	2.02	0.41
1:A:25:GLN:HG2	1:A:73:GLU:HA	2.03	0.41
2:D:58:LEU:HD22	2:D:58:LEU:HA	1.85	0.41
2:D:74:ALA:O	2:D:75:LYS:C	2.64	0.41
2:D:214:MET:C	2:D:216:ASN:H	2.27	0.41
1:E:38:ASP:C	1:E:41:HIS:HB2	2.46	0.41
2:F:37:LYS:O	2:F:37:LYS:CG	2.65	0.41
2:F:43:LYS:HD3	2:F:43:LYS:H	1.85	0.41
2:F:91:VAL:O	2:F:92:ASN:HB2	2.20	0.41
2:H:36:THR:O	2:H:37:LYS:HB3	2.20	0.41
2:B:50:ILE:HD13	2:B:50:ILE:HG21	1.85	0.41
2:B:187:ILE:HA	2:B:193:THR:HG22	2.03	0.41
1:C:36:ARG:HD3	1:C:60:ILE:CD1	2.50	0.41
2:H:129:VAL:CG1	2:H:130:LEU:N	2.83	0.41
1:A:32:MET:HG2	1:A:94:SER:HA	2.03	0.40
2:B:135:GLU:O	2:B:136:ASN:HB2	2.21	0.40
2:D:73:LEU:O	2:D:76:LYS:HB3	2.22	0.40
2:D:221:VAL:HG21	2:D:226:VAL:HG21	2.03	0.40
1:E:32:MET:HG3	1:E:69:ARG:CZ	2.51	0.40
2:F:170:ASN:O	2:F:178:PRO:HD3	2.22	0.40
2:H:70:ASN:OD1	2:H:72:ASP:HB2	2.21	0.40
2:B:100:GLY:C	2:B:102:VAL:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:LEU:HD12	2:F:131:VAL:H	1.86	0.40
2:H:86:GLY:HA3	2:H:155:GLN:OE1	2.18	0.40
2:H:162:ARG:HG2	2:H:198:MET:HE3	2.02	0.40
2:H:166:ILE:HD11	2:H:172:TYR:HD1	1.85	0.40
2:B:21:MET:C	2:B:23:ASN:H	2.29	0.40
2:B:164:PHE:CD2	2:B:164:PHE:C	2.99	0.40
2:B:172:TYR:OH	2:B:198:MET:O	2.27	0.40
2:D:3:GLN:HA	2:D:4:PRO:HD3	1.96	0.40
2:H:103:THR:CG2	2:H:104:GLY:N	2.78	0.40
2:H:174:PHE:HD2	2:H:175:ASN:HD22	1.70	0.40
2:H:207:ASP:O	2:H:208:GLN:C	2.64	0.40
2:B:53:ILE:HB	2:B:64:VAL:HG13	2.03	0.40
2:B:186:PHE:O	2:B:193:THR:HA	2.22	0.40
2:H:84:VAL:HA	2:H:112:GLY:O	2.21	0.40
2:B:188:GLU:C	2:B:190:ASN:N	2.79	0.40
1:C:69:ARG:HG3	1:C:69:ARG:NH2	2.36	0.40
2:F:218:ASN:HD22	2:F:218:ASN:C	2.25	0.40
2:H:82:VAL:HG11	2:H:113:ILE:HG21	2.03	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)
1:A:26:THR:OG1	1:C:26:THR:CG2[1_455]	2.00	0.20

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	105/112 (94%)	91 (87%)	10 (10%)	4 (4%)	2 1
1	C	105/112 (94%)	92 (88%)	9 (9%)	4 (4%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	107/112 (96%)	83 (78%)	16 (15%)	8 (8%)	1	0
1	G	107/112 (96%)	88 (82%)	16 (15%)	3 (3%)	4	2
2	B	232/237 (98%)	188 (81%)	26 (11%)	18 (8%)	1	0
2	D	231/237 (98%)	175 (76%)	34 (15%)	22 (10%)	0	0
2	F	230/237 (97%)	185 (80%)	31 (14%)	14 (6%)	1	0
2	H	233/237 (98%)	167 (72%)	52 (22%)	14 (6%)	1	0
All	All	1350/1396 (97%)	1069 (79%)	194 (14%)	87 (6%)	1	0

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	28	ASN
1	A	39	THR
2	B	80	GLU
2	B	101	LYS
2	B	224	LYS
2	B	225	SER
1	C	27	ASN
2	D	61	TYR
2	D	96	SER
2	D	102	VAL
2	D	125	ASN
1	E	11	LYS
2	F	57	LYS
2	F	219	LYS
2	F	236	ASN
1	G	81	SER
2	H	78	LYS
2	H	123	ASN
2	H	217	ASP
2	H	226	VAL
2	B	8	PRO
2	B	19	GLY
2	B	85	TYR
2	B	102	VAL
2	B	171	LEU
1	C	85	SER
2	D	8	PRO
2	D	75	LYS

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Mol	Chain	Res	Type
2	D	92	ASN
2	D	103	THR
2	D	111	GLY
2	D	124	GLY
2	D	137	LYS
2	D	190	ASN
2	D	226	VAL
1	E	15	THR
1	E	42	GLY
1	E	97	GLY
2	F	25	LYS
2	F	214	MET
2	H	99	ASP
2	H	104	GLY
1	A	108	PHE
2	B	189	ASN
2	B	223	SER
2	D	154	ALA
1	E	82	ALA
1	E	88	SER
2	F	8	PRO
2	F	29	ASP
2	F	92	ASN
2	F	116	HIS
1	G	60	ILE
1	G	110	ALA
2	H	9	ASP
2	H	30	ASP
2	H	219	LYS
2	B	34	SER
2	B	92	ASN
1	C	4	VAL
1	C	30	ASN
2	D	56	LYS
2	D	121	PHE
2	D	191	GLY
1	E	85	SER
2	F	137	LYS
2	F	217	ASP
2	H	37	LYS
2	H	218	ASN
2	B	24	MET

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Mol	Chain	Res	Type
2	B	115	LYS
2	B	121	PHE
2	D	32	TYR
2	D	43	LYS
2	D	116	HIS
2	F	14	SER
2	F	212	LEU
2	H	92	ASN
2	H	236	ASN
2	B	30	ASP
2	D	57	LYS
2	D	74	ALA
2	H	170	ASN
1	E	4	VAL
2	F	141	ILE
2	B	201	ALA

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	88/91 (97%)	75 (85%)	13 (15%)	3	3
1	C	88/91 (97%)	57 (65%)	31 (35%)	0	0
1	E	88/91 (97%)	70 (80%)	18 (20%)	1	1
1	G	88/91 (97%)	61 (69%)	27 (31%)	0	0
2	B	215/217 (99%)	179 (83%)	36 (17%)	2	2
2	D	216/217 (100%)	171 (79%)	45 (21%)	1	1
2	F	215/217 (99%)	156 (73%)	59 (27%)	0	0
2	H	216/217 (100%)	170 (79%)	46 (21%)	1	1
All	All	1214/1232 (98%)	939 (77%)	275 (23%)	1	1

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	11	LYS
1	A	14	VAL
1	A	36	ARG
1	A	54	SER
1	A	57	LYS
1	A	66	LYS
1	A	80	GLU
1	A	87	THR
1	A	89	VAL
1	A	94	SER
1	A	99	THR
1	A	113	ARG
2	B	3	GLN
2	B	7	MET
2	B	24	MET
2	B	40	SER
2	B	41	VAL
2	B	59	LYS
2	B	64	VAL
2	B	68	LEU
2	B	75	LYS
2	B	80	GLU
2	B	88	ASN
2	B	97	SER
2	B	102	VAL
2	B	103	THR
2	B	126	LEU
2	B	132	ARG
2	B	138	ARG
2	B	139	ASN
2	B	141	ILE
2	B	145	VAL
2	B	150	LYS
2	B	166	ILE
2	B	175	ASN
2	B	176	SER
2	B	188	GLU
2	B	189	ASN
2	B	190	ASN
2	B	205	LYS
2	B	209	SER
2	B	212	LEU

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Mol	Chain	Res	Type
2	B	216	ASN
2	B	219	LYS
2	B	224	LYS
2	B	226	VAL
2	B	227	LYS
2	B	234	THR
1	C	7	SER
1	C	9	ARG
1	C	10	ASN
1	C	11	LYS
1	C	15	THR
1	C	18	LYS
1	C	23	CYS
1	C	25	GLN
1	C	26	THR
1	C	27	ASN
1	C	33	TYR
1	C	37	GLN
1	C	43	LEU
1	C	44	ARG
1	C	49	SER
1	C	55	THR
1	C	56	GLU
1	C	68	SER
1	C	69	ARG
1	C	71	SER
1	C	72	GLN
1	C	73	GLU
1	C	77	LEU
1	C	81	SER
1	C	83	THR
1	C	85	SER
1	C	87	THR
1	C	88	SER
1	C	92	CYS
1	C	108	PHE
1	C	113	ARG
2	D	3	GLN
2	D	20	THR
2	D	34	SER
2	D	36	THR
2	D	37	LYS

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Mol	Chain	Res	Type
2	D	56	LYS
2	D	57	LYS
2	D	58	LEU
2	D	65	LYS
2	D	68	LEU
2	D	72	ASP
2	D	73	LEU
2	D	87	SER
2	D	88	ASN
2	D	93	CYS
2	D	96	SER
2	D	99	ASP
2	D	101	LYS
2	D	102	VAL
2	D	106	LYS
2	D	109	MET
2	D	115	LYS
2	D	117	GLU
2	D	125	ASN
2	D	132	ARG
2	D	135	GLU
2	D	138	ARG
2	D	139	ASN
2	D	141	ILE
2	D	144	GLU
2	D	157	LEU
2	D	162	ARG
2	D	168	LYS
2	D	169	LYS
2	D	175	ASN
2	D	177	SER
2	D	194	PHE
2	D	204	ASP
2	D	213	MET
2	D	216	ASN
2	D	219	LYS
2	D	220	THR
2	D	222	ASP
2	D	224	LYS
2	D	233	THR
1	E	14	VAL
1	E	27	ASN

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Mol	Chain	Res	Type
1	E	28	ASN
1	E	32	MET
1	E	37	GLN
1	E	43	LEU
1	E	44	ARG
1	E	49	SER
1	E	50	TYR
1	E	55	THR
1	E	60	ILE
1	E	61	PRO
1	E	68	SER
1	E	74	GLN
1	E	85	SER
1	E	88	SER
1	E	99	THR
1	E	117	LEU
2	F	2	SER
2	F	3	GLN
2	F	7	MET
2	F	9	ASP
2	F	10	ASP
2	F	20	THR
2	F	34	SER
2	F	37	LYS
2	F	39	LYS
2	F	42	ASP
2	F	43	LYS
2	F	53	ILE
2	F	54	SER
2	F	56	LYS
2	F	57	LYS
2	F	58	LEU
2	F	59	LYS
2	F	72	ASP
2	F	73	LEU
2	F	76	LYS
2	F	80	GLU
2	F	82	VAL
2	F	84	VAL
2	F	90	TYR
2	F	92	ASN
2	F	97	SER

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Mol	Chain	Res	Type
2	F	103	THR
2	F	109	MET
2	F	115	LYS
2	F	117	GLU
2	F	123	ASN
2	F	126	LEU
2	F	129	VAL
2	F	140	THR
2	F	141	ILE
2	F	145	VAL
2	F	150	LYS
2	F	151	SER
2	F	157	LEU
2	F	166	ILE
2	F	168	LYS
2	F	169	LYS
2	F	170	ASN
2	F	175	ASN
2	F	176	SER
2	F	180	GLU
2	F	184	ILE
2	F	194	PHE
2	F	198	MET
2	F	205	LYS
2	F	216	ASN
2	F	218	ASN
2	F	224	LYS
2	F	225	SER
2	F	228	ILE
2	F	233	THR
2	F	234	THR
2	F	235	LYS
2	F	236	ASN
1	G	4	VAL
1	G	6	GLN
1	G	9	ARG
1	G	14	VAL
1	G	15	THR
1	G	17	GLU
1	G	18	LYS
1	G	19	VAL
1	G	21	LEU

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Mol	Chain	Res	Type
1	G	25	GLN
1	G	26	THR
1	G	29	HIS
1	G	31	ASN
1	G	41	HIS
1	G	43	LEU
1	G	44	ARG
1	G	46	ILE
1	G	49	SER
1	G	55	THR
1	G	57	LYS
1	G	59	ASP
1	G	60	ILE
1	G	79	LEU
1	G	86	GLN
1	G	89	VAL
1	G	92	CYS
1	G	99	THR
2	H	2	SER
2	H	7	MET
2	H	9	ASP
2	H	33	VAL
2	H	34	SER
2	H	37	LYS
2	H	39	LYS
2	H	43	LYS
2	H	56	LYS
2	H	57	LYS
2	H	67	GLU
2	H	69	LEU
2	H	73	LEU
2	H	75	LYS
2	H	79	ASP
2	H	82	VAL
2	H	87	SER
2	H	88	ASN
2	H	97	SER
2	H	109	MET
2	H	113	ILE
2	H	122	ASP
2	H	140	THR
2	H	142	SER

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Mol	Chain	Res	Type
2	H	147	THR
2	H	150	LYS
2	H	151	SER
2	H	170	ASN
2	H	175	ASN
2	H	176	SER
2	H	181	THR
2	H	184	ILE
2	H	187	ILE
2	H	188	GLU
2	H	189	ASN
2	H	190	ASN
2	H	209	SER
2	H	214	MET
2	H	216	ASN
2	H	218	ASN
2	H	220	THR
2	H	225	SER
2	H	227	LYS
2	H	229	GLU
2	H	233	THR
2	H	236	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	ASN
1	A	74	GLN
2	B	31	HIS
2	B	88	ASN
2	B	139	ASN
2	B	146	GLN
2	B	155	GLN
2	B	175	ASN
2	B	189	ASN
2	B	190	ASN
2	B	216	ASN
1	C	28	ASN
1	C	30	ASN
1	C	37	GLN
1	C	72	GLN

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Mol	Chain	Res	Type
1	C	74	GLN
2	D	3	GLN
2	D	31	HIS
2	D	47	HIS
2	D	88	ASN
2	D	92	ASN
2	D	127	GLN
2	D	136	ASN
2	D	167	ASN
2	D	175	ASN
2	D	216	ASN
1	E	24	GLN
2	F	3	GLN
2	F	88	ASN
2	F	92	ASN
2	F	116	HIS
2	F	127	GLN
2	F	216	ASN
2	F	236	ASN
1	G	31	ASN
1	G	37	GLN
1	G	41	HIS
2	H	31	HIS
2	H	88	ASN
2	H	120	HIS
2	H	128	ASN
2	H	136	ASN
2	H	170	ASN
2	H	189	ASN
2	H	216	ASN
2	H	236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	A	2
1	E	2
2	H	1
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	101:LYS	C	102:VAL	N	7.11
1	C	101:TYR	C	108:PHE	N	2.52
1	A	63:GLY	C	65:TYR	N	2.04
1	A	101:TYR	C	108:PHE	N	1.87
1	E	101:TYR	C	108:PHE	N	1.83
1	C	63:GLY	C	65:TYR	N	1.80
1	E	63:GLY	C	65:TYR	N	1.76
1	G	101:TYR	C	108:PHE	N	1.74

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	109/112 (97%)	-0.26	0 100 100	8, 35, 52, 59	0
1	C	109/112 (97%)	-0.15	1 (0%) 81 82	21, 39, 58, 66	0
1	E	109/112 (97%)	-0.03	1 (0%) 81 82	27, 47, 64, 70	0
1	G	109/112 (97%)	-0.11	1 (0%) 81 82	24, 40, 59, 63	0
2	B	234/237 (98%)	-0.20	2 (0%) 81 82	10, 41, 65, 86	0
2	D	235/237 (99%)	-0.00	3 (1%) 75 76	23, 47, 71, 87	0
2	F	234/237 (98%)	-0.06	0 100 100	29, 45, 75, 91	0
2	H	237/237 (100%)	0.10	6 (2%) 58 60	27, 50, 76, 103	0
All	All	1376/1396 (98%)	-0.07	14 (1%) 79 80	8, 44, 69, 103	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	101	LYS	3.6
2	D	102	VAL	3.3
2	H	102	VAL	3.1
2	B	102	VAL	2.8
2	H	237	GLY	2.8
2	H	103	THR	2.7
2	B	105	GLY	2.5
2	H	100	GLY	2.5
2	D	237	GLY	2.4
2	H	104	GLY	2.3
1	E	3	ALA	2.3
1	C	2	ALA	2.2
1	G	3	ALA	2.0
2	D	97	SER	2.0

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

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.