Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:35 AM GMT

PDB ID	:	2AQ3
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

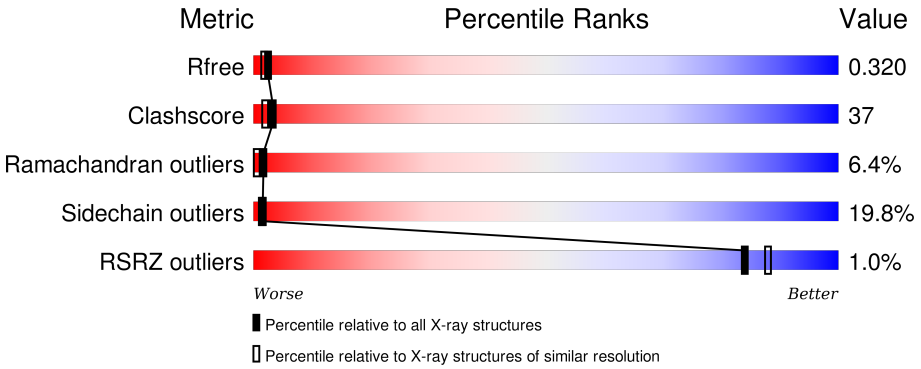
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	% 25% 39% 29%
1	C	112	% 27% 33% 31% 6%
1	E	112	% 40% 38% 18%
1	G	112	29% 48% 17%
2	B	237	34% 37% 23% 5%

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Mol	Chain	Length	Quality of chain
2	D	237	2% 30% 48% 19%
2	F	237	27% 48% 18% 6%
2	H	237	2% 34% 43% 18% 5%

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.

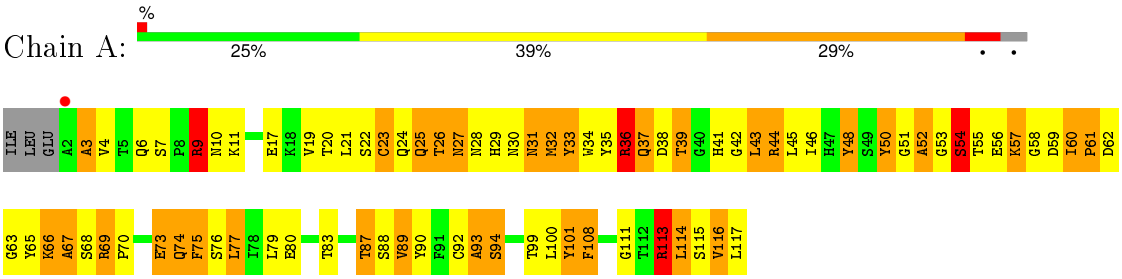
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	21	Total O 21 21	0	0
3	B	48	Total O 48 48	0	0
3	C	15	Total O 15 15	0	0
3	D	31	Total O 31 31	0	0
3	E	11	Total O 11 11	0	0
3	F	31	Total O 31 31	0	0
3	G	15	Total O 15 15	0	0
3	H	26	Total O 26 26	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

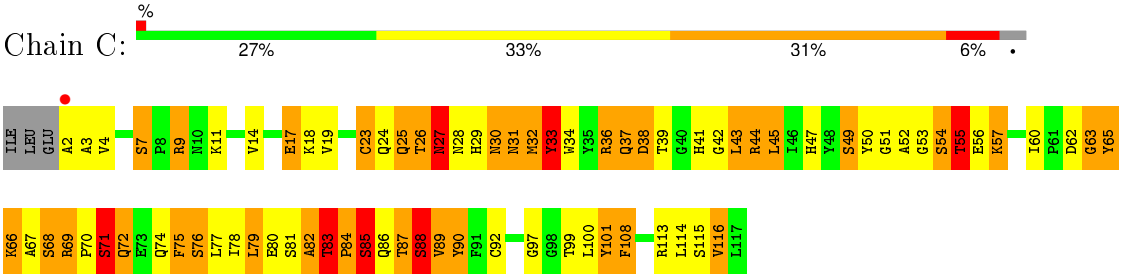
- Molecule 1: T-cell receptor beta chain V

Chain A:



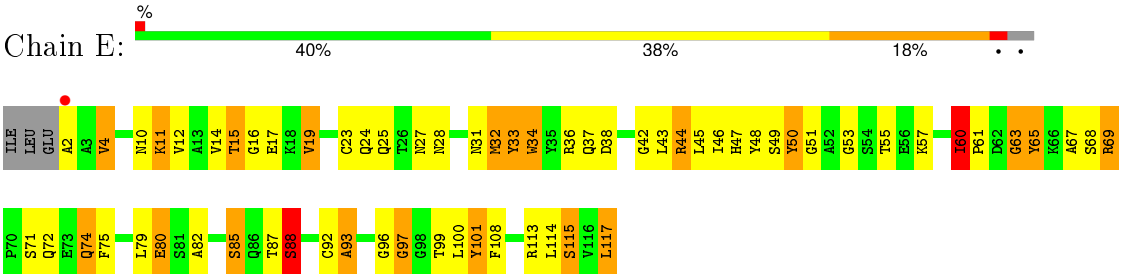
- Molecule 1: T-cell receptor beta chain V

Chain C:



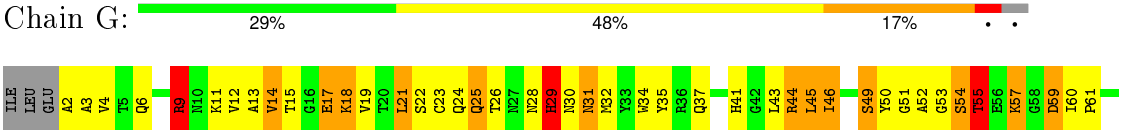
- Molecule 1: T-cell receptor beta chain V

Chain E:



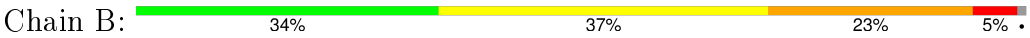
- Molecule 1: T-cell receptor beta chain V

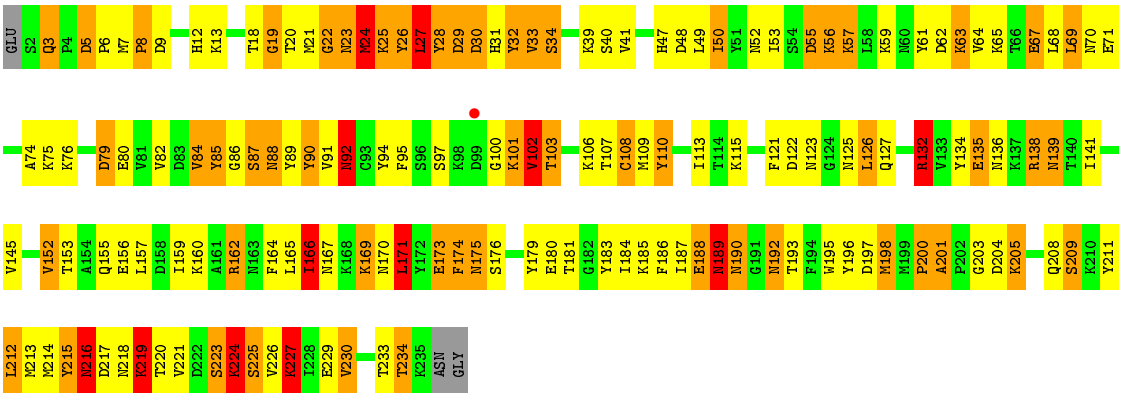
Chain G:



• Molecule 2: Enterotoxin type C-3

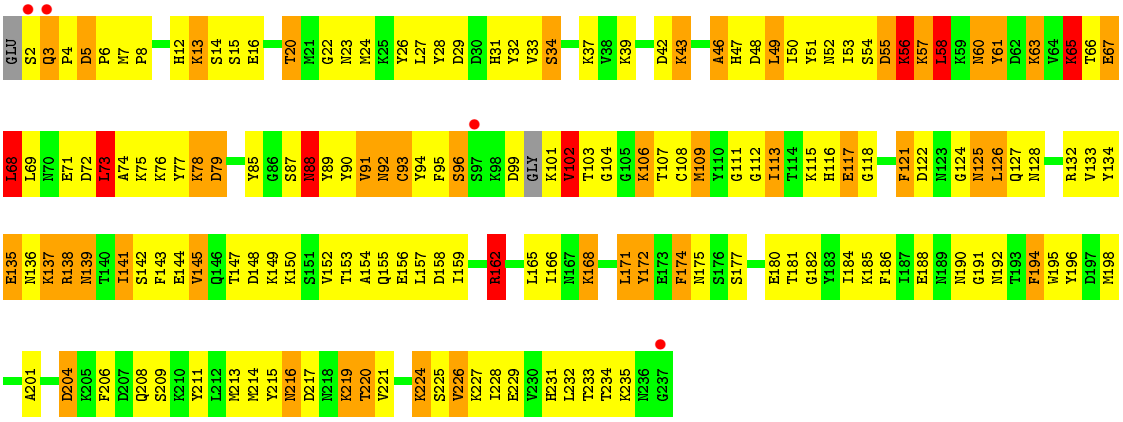
Chain B:





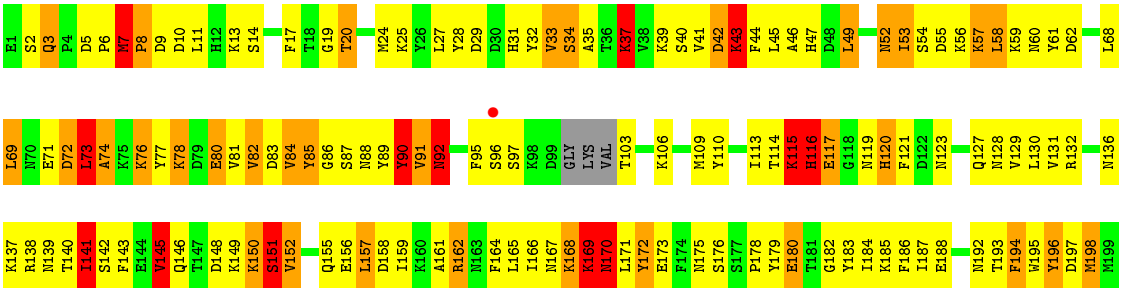
• Molecule 2: Enterotoxin type C-3

Chain D:

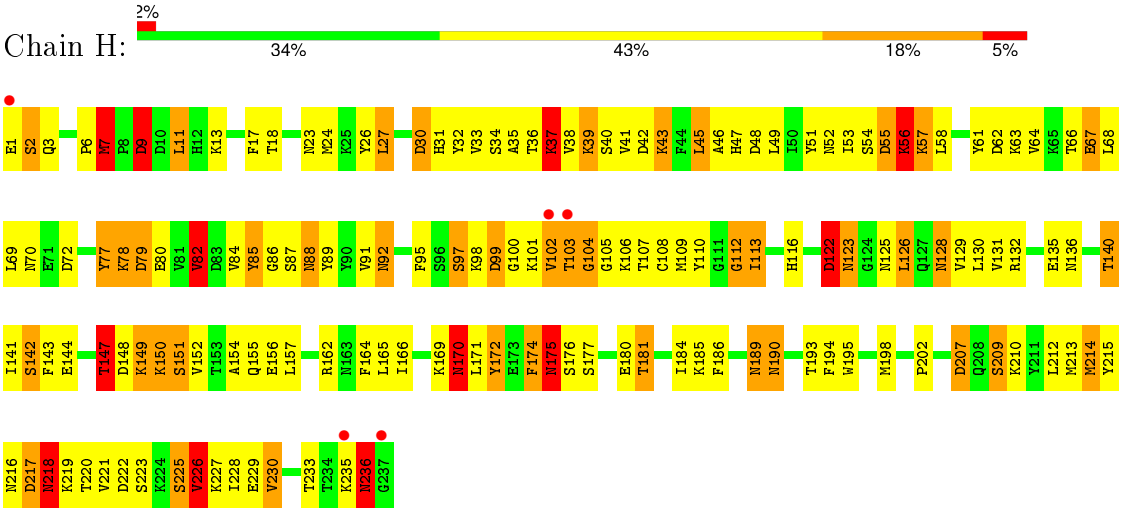


• Molecule 2: Enterotoxin type C-3

Chain F:



• Molecule 2: Enterotoxin type C-3



4 Data and refinement statistics (i)

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 63.42 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-2.30) 85.5 (63.42-2.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	3394 reflections (5.32%)	DCC
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 , 66.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 67372 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	2.51	38/845 (4.5%)	2.06	26/1142 (2.3%)
1	C	2.25	31/845 (3.7%)	1.88	19/1142 (1.7%)
1	E	2.20	24/846 (2.8%)	1.74	15/1145 (1.3%)
1	G	2.13	15/846 (1.8%)	1.98	22/1145 (1.9%)
2	B	2.05	63/1945 (3.2%)	1.72	37/2619 (1.4%)
2	D	1.83	26/1953 (1.3%)	1.67	32/2627 (1.2%)
2	F	1.83	31/1946 (1.6%)	1.60	22/2618 (0.8%)
2	H	1.77	30/1962 (1.5%)	1.56	22/2640 (0.8%)
All	All	2.00	258/11188 (2.3%)	1.73	195/15078 (1.3%)

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 (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	TYR	C-N	23.04	1.87	1.34
1	E	101	TYR	C-N	21.36	1.83	1.34
1	C	63	GLY	C-N	20.06	1.80	1.34
1	E	63	GLY	C-N	18.65	1.76	1.34
1	G	101	TYR	C-N	17.43	1.74	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	80	GLU	CG-CD	15.86	1.75	1.51
2	H	172	TYR	CE1-CZ	13.55	1.56	1.38
1	A	33	TYR	CD2-CE2	13.12	1.59	1.39
1	C	80	GLU	CG-CD	11.17	1.68	1.51
2	B	26	TYR	CB-CG	11.04	1.68	1.51
2	D	172	TYR	CE2-CZ	10.57	1.52	1.38
1	A	56	GLU	CB-CG	10.55	1.72	1.52
1	G	80	GLU	CG-CD	10.46	1.67	1.51
1	A	53	GLY	N-CA	-10.42	1.30	1.46
1	G	65	TYR	C-O	10.01	1.42	1.23
2	H	32	TYR	CD1-CE1	-9.99	1.24	1.39
2	D	89	TYR	CD2-CE2	-9.96	1.24	1.39
2	D	172	TYR	CD1-CE1	9.75	1.53	1.39
1	G	65	TYR	CE2-CZ	9.59	1.51	1.38
2	B	164	PHE	CE1-CZ	9.52	1.55	1.37
2	B	27	LEU	CG-CD1	9.43	1.86	1.51
1	A	67	ALA	CA-CB	-9.38	1.32	1.52
1	G	52	ALA	CA-CB	9.28	1.72	1.52
1	A	54	SER	CB-OG	9.10	1.54	1.42
1	C	80	GLU	CD-OE2	8.97	1.35	1.25
1	C	23	CYS	CB-SG	-8.61	1.67	1.82
1	A	52	ALA	CA-CB	8.60	1.70	1.52
1	G	80	GLU	CD-OE2	8.58	1.35	1.25
2	B	26	TYR	CG-CD2	8.51	1.50	1.39
1	E	92	CYS	CB-SG	-8.31	1.68	1.82
2	B	110	TYR	CD1-CE1	8.28	1.51	1.39
2	B	174	PHE	CE1-CZ	-8.21	1.21	1.37
2	B	26	TYR	N-CA	8.19	1.62	1.46
1	A	75	PHE	CG-CD1	-8.12	1.26	1.38
1	C	82	ALA	CA-CB	-8.10	1.35	1.52
1	C	52	ALA	CA-CB	8.10	1.69	1.52
2	D	22	GLY	C-O	7.97	1.36	1.23
2	H	82	VAL	CB-CG1	7.94	1.69	1.52
2	D	211	TYR	CD1-CE1	7.86	1.51	1.39
2	H	172	TYR	CG-CD1	7.84	1.49	1.39
2	F	211	TYR	CD2-CE2	-7.78	1.27	1.39
2	B	215	TYR	CD1-CE1	7.76	1.50	1.39
1	E	80	GLU	CB-CG	7.60	1.66	1.52
1	A	90	TYR	CD1-CE1	7.59	1.50	1.39
2	B	91	VAL	CB-CG1	-7.59	1.36	1.52
2	D	65	LYS	CD-CE	7.54	1.70	1.51
2	B	27	LEU	N-CA	7.52	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	GLU	CG-CD	7.45	1.63	1.51
2	B	63	LYS	CD-CE	7.39	1.69	1.51
2	B	205	LYS	CD-CE	7.32	1.69	1.51
1	A	26	THR	CB-CG2	7.24	1.76	1.52
1	A	19	VAL	CB-CG1	-7.22	1.37	1.52
2	F	215	TYR	CD1-CE1	7.17	1.50	1.39
1	G	45	LEU	C-O	7.13	1.36	1.23
1	A	76	SER	CB-OG	7.08	1.51	1.42
2	F	179	TYR	CD1-CE1	7.04	1.50	1.39
2	B	110	TYR	CE1-CZ	7.01	1.47	1.38
2	F	152	VAL	CB-CG2	-6.97	1.38	1.52
1	C	19	VAL	CA-CB	6.95	1.69	1.54
1	E	65	TYR	CD2-CE2	6.91	1.49	1.39
2	B	94	TYR	CD1-CE1	6.87	1.49	1.39
2	F	173	GLU	CD-OE1	6.86	1.33	1.25
2	H	156	GLU	CG-CD	6.84	1.62	1.51
2	B	152	VAL	CB-CG2	-6.81	1.38	1.52
2	B	173	GLU	C-O	6.81	1.36	1.23
2	B	200	PRO	N-CA	-6.80	1.35	1.47
2	D	186	PHE	CE2-CZ	6.80	1.50	1.37
2	B	87	SER	CB-OG	-6.78	1.33	1.42
2	F	28	TYR	CD1-CE1	6.76	1.49	1.39
2	B	24	MET	C-O	6.75	1.36	1.23
2	F	151	SER	CB-OG	6.74	1.51	1.42
2	D	196	TYR	CE2-CZ	-6.71	1.29	1.38
1	E	48	TYR	CD1-CE1	6.70	1.49	1.39
2	B	229	GLU	CD-OE1	6.69	1.33	1.25
1	G	101	TYR	CG-CD2	6.69	1.47	1.39
1	A	76	SER	N-CA	6.67	1.59	1.46
1	C	85	SER	CB-OG	6.63	1.50	1.42
2	B	33	VAL	CB-CG2	-6.62	1.39	1.52
1	E	34	TRP	CB-CG	6.62	1.62	1.50
1	E	50	TYR	CE1-CZ	6.61	1.47	1.38
1	A	56	GLU	CG-CD	-6.59	1.42	1.51
2	D	162	ARG	CG-CD	6.58	1.68	1.51
1	A	30	ASN	CB-CG	6.58	1.66	1.51
2	B	221	VAL	CB-CG2	6.57	1.66	1.52
1	C	88	SER	CB-OG	6.56	1.50	1.42
1	G	108	PHE	CD1-CE1	6.53	1.52	1.39
2	H	26	TYR	CD1-CE1	-6.52	1.29	1.39
2	H	77	TYR	CD2-CE2	6.51	1.49	1.39
1	C	53	GLY	N-CA	6.45	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	215	TYR	CD2-CE2	6.38	1.49	1.39
1	C	116	VAL	CA-CB	-6.37	1.41	1.54
1	C	101	TYR	CD2-CE2	-6.36	1.29	1.39
1	E	57	LYS	CE-NZ	6.33	1.64	1.49
1	C	38	ASP	CB-CG	6.33	1.65	1.51
2	H	101	LYS	CA-CB	6.33	1.67	1.53
1	E	51	GLY	N-CA	6.32	1.55	1.46
2	B	82	VAL	CB-CG1	6.31	1.66	1.52
1	E	50	TYR	CZ-OH	6.31	1.48	1.37
2	B	57	LYS	CD-CE	6.29	1.67	1.51
2	B	174	PHE	CD1-CE1	-6.29	1.26	1.39
2	F	208	GLN	C-O	6.27	1.35	1.23
2	F	162	ARG	CG-CD	6.23	1.67	1.51
2	B	89	TYR	CZ-OH	-6.23	1.27	1.37
2	F	78	LYS	CD-CE	6.23	1.66	1.51
2	D	172	TYR	CG-CD1	6.18	1.47	1.39
2	F	43	LYS	CD-CE	6.16	1.66	1.51
2	H	103	THR	CA-CB	6.12	1.69	1.53
2	B	27	LEU	C-O	6.10	1.34	1.23
1	G	66	LYS	CA-CB	-6.09	1.40	1.53
2	H	102	VAL	CA-CB	6.07	1.67	1.54
1	C	71	SER	CB-OG	6.06	1.50	1.42
2	F	77	TYR	CD1-CE1	-6.05	1.30	1.39
1	C	45	LEU	N-CA	6.05	1.58	1.46
1	E	80	GLU	CD-OE2	6.05	1.32	1.25
1	C	76	SER	CB-OG	-6.03	1.34	1.42
1	A	25	GLN	CD-NE2	6.03	1.48	1.32
1	A	116	VAL	CB-CG1	-6.02	1.40	1.52
1	E	2	ALA	CA-CB	6.02	1.65	1.52
1	C	80	GLU	CD-OE1	6.02	1.32	1.25
1	A	60	ILE	CA-CB	6.02	1.68	1.54
2	B	102	VAL	CA-CB	6.00	1.67	1.54
2	D	93	CYS	CB-SG	-6.00	1.72	1.82
2	B	32	TYR	CE1-CZ	5.99	1.46	1.38
2	B	192	ASN	N-CA	5.99	1.58	1.46
1	A	55	THR	CB-CG2	5.98	1.72	1.52
2	B	216	ASN	CB-CG	-5.97	1.37	1.51
2	H	175	ASN	CB-CG	5.97	1.64	1.51
1	G	101	TYR	CE2-CZ	5.95	1.46	1.38
1	C	17	GLU	CD-OE1	5.95	1.32	1.25
2	F	115	LYS	CB-CG	5.92	1.68	1.52
2	H	17	PHE	CD1-CE1	-5.92	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	164	PHE	CG-CD1	5.90	1.47	1.38
2	B	22	GLY	N-CA	5.89	1.54	1.46
2	B	230	VAL	CB-CG1	-5.87	1.40	1.52
1	E	80	GLU	CA-CB	5.87	1.66	1.53
2	B	28	TYR	CZ-OH	-5.87	1.27	1.37
1	C	34	TRP	CG-CD1	-5.84	1.28	1.36
1	A	27	ASN	CB-CG	5.84	1.64	1.51
2	D	132	ARG	CG-CD	5.81	1.66	1.51
2	H	46	ALA	CA-CB	5.80	1.64	1.52
1	E	67	ALA	CA-CB	5.79	1.64	1.52
1	A	54	SER	CA-CB	5.77	1.61	1.52
1	A	51	GLY	N-CA	5.76	1.54	1.46
2	H	85	TYR	CZ-OH	5.75	1.47	1.37
1	C	2	ALA	CA-CB	5.75	1.64	1.52
2	H	230	VAL	CB-CG1	-5.74	1.40	1.52
2	D	91	VAL	C-O	5.73	1.34	1.23
2	F	218	ASN	CA-C	5.73	1.67	1.52
2	B	166	ILE	CA-C	5.72	1.67	1.52
2	B	227	LYS	CE-NZ	5.72	1.63	1.49
1	A	53	GLY	CA-C	-5.72	1.42	1.51
2	B	196	TYR	CG-CD2	5.72	1.46	1.39
2	F	145	VAL	CA-CB	5.70	1.66	1.54
2	B	26	TYR	CE2-CZ	5.69	1.46	1.38
2	D	174	PHE	CD1-CE1	-5.68	1.27	1.39
2	H	9	ASP	CB-CG	5.67	1.63	1.51
2	B	196	TYR	CD1-CE1	-5.67	1.30	1.39
2	F	205	LYS	CD-CE	5.67	1.65	1.51
2	D	46	ALA	CA-CB	5.67	1.64	1.52
2	B	90	TYR	CE1-CZ	5.66	1.46	1.38
2	F	215	TYR	CE1-CZ	5.65	1.45	1.38
2	B	164	PHE	C-O	-5.65	1.12	1.23
2	F	142	SER	CB-OG	5.64	1.49	1.42
1	A	75	PHE	CA-C	5.63	1.67	1.52
2	D	67	GLU	CG-CD	5.63	1.60	1.51
2	F	85	TYR	CE1-CZ	5.61	1.45	1.38
2	B	67	GLU	CG-CD	-5.60	1.43	1.51
2	H	164	PHE	CB-CG	5.60	1.60	1.51
2	H	1	GLU	CG-CD	5.59	1.60	1.51
1	E	33	TYR	CB-CG	-5.59	1.43	1.51
2	F	37	LYS	CD-CE	5.58	1.65	1.51
2	B	63	LYS	CE-NZ	5.57	1.62	1.49
2	D	145	VAL	CA-CB	5.57	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	76	LYS	C-O	5.57	1.33	1.23
2	D	162	ARG	CZ-NH2	5.55	1.40	1.33
1	C	53	GLY	C-O	5.54	1.32	1.23
1	A	32	MET	SD-CE	5.53	2.08	1.77
2	B	61	TYR	CG-CD1	-5.51	1.31	1.39
1	G	108	PHE	CE2-CZ	5.50	1.47	1.37
2	F	72	ASP	CB-CG	5.48	1.63	1.51
2	F	161	ALA	CA-CB	5.47	1.64	1.52
2	B	108	CYS	CB-SG	-5.47	1.72	1.81
1	A	90	TYR	CE2-CZ	5.47	1.45	1.38
2	H	77	TYR	CG-CD2	5.46	1.46	1.39
2	B	229	GLU	C-O	-5.46	1.12	1.23
1	A	53	GLY	C-O	5.46	1.32	1.23
2	B	171	LEU	C-O	5.45	1.33	1.23
2	B	84	VAL	CB-CG2	-5.44	1.41	1.52
2	D	172	TYR	C-O	5.44	1.33	1.23
1	E	50	TYR	CD2-CE2	5.42	1.47	1.39
1	C	54	SER	CB-OG	5.42	1.49	1.42
1	E	50	TYR	CE2-CZ	5.42	1.45	1.38
2	F	46	ALA	CA-CB	5.42	1.63	1.52
1	A	17	GLU	CG-CD	5.41	1.60	1.51
2	F	78	LYS	CB-CG	5.40	1.67	1.52
1	A	48	TYR	CE1-CZ	5.39	1.45	1.38
1	G	53	GLY	N-CA	-5.38	1.38	1.46
2	D	108	CYS	CB-SG	-5.37	1.73	1.81
2	B	29	ASP	C-O	-5.36	1.13	1.23
1	E	51	GLY	CA-C	5.35	1.60	1.51
2	H	164	PHE	CE2-CZ	5.35	1.47	1.37
1	A	48	TYR	CG-CD1	5.35	1.46	1.39
2	F	90	TYR	CD2-CE2	-5.34	1.31	1.39
1	C	90	TYR	CD1-CE1	5.33	1.47	1.39
2	B	219	LYS	CG-CD	5.33	1.70	1.52
1	A	50	TYR	CD2-CE2	5.32	1.47	1.39
2	H	174	PHE	CD2-CE2	-5.32	1.28	1.39
2	F	196	TYR	CD2-CE2	5.31	1.47	1.39
1	A	50	TYR	CZ-OH	5.30	1.46	1.37
1	C	71	SER	N-CA	5.30	1.56	1.46
2	B	215	TYR	CE1-CZ	-5.29	1.31	1.38
2	F	17	PHE	CE1-CZ	-5.29	1.27	1.37
2	F	185	LYS	CD-CE	5.28	1.64	1.51
1	G	108	PHE	C-O	5.28	1.33	1.23
2	F	200	PRO	C-O	5.27	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	154	ALA	CA-CB	5.27	1.63	1.52
1	A	44	ARG	CB-CG	5.26	1.66	1.52
1	A	73	GLU	CD-OE2	5.25	1.31	1.25
1	E	19	VAL	CA-CB	5.23	1.65	1.54
1	C	66	LYS	CG-CD	5.21	1.70	1.52
1	E	50	TYR	CB-CG	5.21	1.59	1.51
2	H	56	LYS	CB-CG	5.21	1.66	1.52
2	B	25	LYS	N-CA	5.20	1.56	1.46
2	B	74	ALA	CA-CB	-5.19	1.41	1.52
2	B	169	LYS	C-O	5.19	1.33	1.23
1	E	80	GLU	CD-OE1	5.18	1.31	1.25
1	A	37	GLN	N-CA	5.18	1.56	1.46
2	D	26	TYR	CE2-CZ	-5.18	1.31	1.38
1	A	74	GLN	CA-CB	-5.18	1.42	1.53
2	B	28	TYR	N-CA	5.17	1.56	1.46
1	G	101	TYR	CD2-CE2	5.17	1.47	1.39
2	B	27	LEU	CG-CD2	5.16	1.71	1.51
2	B	135	GLU	CD-OE1	-5.13	1.20	1.25
2	B	224	LYS	CD-CE	5.13	1.64	1.51
1	C	84	PRO	N-CA	5.12	1.55	1.47
2	D	171	LEU	C-O	5.12	1.33	1.23
2	H	32	TYR	CD2-CE2	-5.11	1.31	1.39
1	C	66	LYS	CE-NZ	5.10	1.61	1.49
2	D	209	SER	CB-OG	5.10	1.48	1.42
2	B	87	SER	N-CA	-5.09	1.36	1.46
1	A	20	THR	CB-CG2	5.07	1.69	1.52
1	C	83	THR	N-CA	5.07	1.56	1.46
2	D	201	ALA	CA-CB	-5.04	1.41	1.52
2	H	149	LYS	CE-NZ	5.04	1.61	1.49
2	B	214	MET	N-CA	-5.04	1.36	1.46
2	H	164	PHE	CD1-CE1	5.04	1.49	1.39
2	B	159	ILE	CA-CB	-5.03	1.43	1.54
1	C	65	TYR	CE1-CZ	5.03	1.45	1.38
1	C	65	TYR	CE2-CZ	-5.03	1.32	1.38
2	B	183	TYR	CZ-OH	5.03	1.46	1.37
2	F	91	VAL	C-O	5.02	1.32	1.23
2	H	27	LEU	N-CA	5.02	1.56	1.46
2	B	229	GLU	CD-OE2	5.02	1.31	1.25
2	H	100	GLY	CA-C	5.02	1.59	1.51
1	A	23	CYS	CB-SG	5.01	1.90	1.82
1	C	33	TYR	CD2-CE2	-5.01	1.31	1.39
1	E	48	TYR	CE1-CZ	-5.00	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	172	TYR	CG-CD2	5.00	1.45	1.39

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	101	TYR	O-C-N	-23.91	84.44	122.70
1	A	101	TYR	O-C-N	-22.11	87.32	122.70
1	E	101	TYR	O-C-N	-18.64	92.88	122.70
2	D	162	ARG	NE-CZ-NH1	-16.09	112.25	120.30
2	D	29	ASP	CB-CG-OD1	-13.04	106.57	118.30
2	B	55	ASP	CB-CG-OD1	12.85	129.86	118.30
1	C	79	LEU	CB-CG-CD1	12.54	132.31	111.00
2	B	165	LEU	CB-CG-CD2	-11.18	92.00	111.00
2	F	24	MET	CG-SD-CE	-11.08	82.47	100.20
2	D	29	ASP	CB-CG-OD2	10.50	127.75	118.30
1	G	79	LEU	CA-CB-CG	10.29	138.97	115.30
1	A	36	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	C	36	ARG	NE-CZ-NH2	-9.43	115.59	120.30
2	D	5	ASP	CB-CG-OD2	-9.38	109.86	118.30
2	B	122	ASP	CB-CG-OD1	9.18	126.56	118.30
1	A	36	ARG	NE-CZ-NH2	9.12	124.86	120.30
2	F	73	LEU	CA-CB-CG	9.12	136.28	115.30
1	A	92	CYS	CA-CB-SG	-8.92	97.94	114.00
2	B	55	ASP	CB-CG-OD2	-8.90	110.29	118.30
2	B	5	ASP	CB-CG-OD2	8.68	126.11	118.30
2	F	49	LEU	CA-CB-CG	8.55	134.96	115.30
1	A	77	LEU	CB-CG-CD2	-8.53	96.49	111.00
2	H	217	ASP	CB-CG-OD1	8.45	125.91	118.30
2	D	162	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	E	63	GLY	CA-C-N	-8.30	98.94	117.20
2	B	5	ASP	CB-CG-OD1	-8.15	110.96	118.30
2	B	126	LEU	CB-CG-CD1	-8.15	97.14	111.00
2	H	45	LEU	CB-CG-CD2	-7.76	97.81	111.00
2	D	214	MET	CG-SD-CE	-7.76	87.79	100.20
2	D	49	LEU	CB-CG-CD2	-7.74	97.84	111.00
1	E	63	GLY	O-C-N	-7.69	110.39	122.70
1	E	69	ARG	NE-CZ-NH2	-7.67	116.47	120.30
2	D	149	LYS	N-CA-C	-7.57	90.58	111.00
1	A	113	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	G	66	LYS	CD-CE-NZ	-7.50	94.45	111.70
1	A	69	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	B	24	MET	N-CA-C	7.40	130.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	GLN	CB-CA-C	-7.33	95.75	110.40
1	C	79	LEU	CB-CG-CD2	-7.21	98.73	111.00
1	C	97	GLY	N-CA-C	-7.16	95.19	113.10
1	A	114	LEU	CB-CG-CD2	7.14	123.14	111.00
2	H	207	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	43	LEU	CB-CG-CD2	-6.98	99.14	111.00
1	E	101	TYR	C-N-CA	-6.97	104.27	121.70
1	C	32	MET	CB-CG-SD	6.97	133.30	112.40
2	F	222	ASP	CB-CG-OD2	-6.91	112.08	118.30
2	H	45	LEU	CA-CB-CG	6.90	131.17	115.30
2	D	68	LEU	CA-CB-CG	6.85	131.05	115.30
2	H	52	ASN	CB-CA-C	-6.81	96.78	110.40
1	C	23	CYS	CA-CB-SG	6.80	126.25	114.00
1	C	76	SER	N-CA-CB	-6.75	100.37	110.50
2	F	69	LEU	CA-CB-CG	6.73	130.79	115.30
1	A	21	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	A	79	LEU	CA-CB-CG	6.69	130.69	115.30
1	E	113	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	D	126	LEU	CA-CB-CG	6.59	130.47	115.30
1	E	60	ILE	C-N-CD	6.58	142.22	128.40
2	F	222	ASP	CB-CG-OD1	6.55	124.19	118.30
2	F	170	ASN	N-CA-CB	6.49	122.28	110.60
2	H	30	ASP	CB-CG-OD2	6.48	124.13	118.30
2	B	79	ASP	CB-CG-OD1	-6.48	112.47	118.30
2	B	157	LEU	CB-CG-CD1	-6.47	100.00	111.00
2	B	28	TYR	CD1-CE1-CZ	-6.46	113.99	119.80
2	D	113	ILE	CB-CA-C	-6.45	98.69	111.60
2	B	196	TYR	CB-CG-CD1	-6.43	117.14	121.00
2	B	50	ILE	CG1-CB-CG2	-6.40	97.33	111.40
2	B	196	TYR	CA-CB-CG	6.38	125.52	113.40
2	H	41	VAL	CG1-CB-CG2	-6.38	100.70	110.90
1	G	45	LEU	CA-CB-CG	6.32	129.84	115.30
2	H	147	THR	CB-CA-C	-6.30	94.59	111.60
1	G	111	GLY	N-CA-C	6.24	128.69	113.10
1	G	96	GLY	N-CA-C	-6.23	97.52	113.10
2	D	13	LYS	CD-CE-NZ	-6.23	97.37	111.70
1	C	62	ASP	CB-CG-OD1	6.20	123.88	118.30
2	F	196	TYR	CB-CG-CD2	6.20	124.72	121.00
2	D	217	ASP	CB-CG-OD1	6.19	123.87	118.30
2	B	216	ASN	CB-CA-C	-6.18	98.03	110.40
1	G	79	LEU	CB-CG-CD2	-6.18	100.50	111.00
2	H	58	LEU	N-CA-C	-6.11	94.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	68	LEU	CA-CB-CG	-6.11	101.24	115.30
2	D	148	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	F	72	ASP	CB-CG-OD1	6.09	123.78	118.30
2	F	171	LEU	CB-CG-CD1	6.09	121.36	111.00
2	B	145	VAL	CB-CA-C	6.08	122.96	111.40
1	A	9	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	D	90	TYR	N-CA-C	-6.06	94.65	111.00
2	D	204	ASP	CB-CG-OD2	-6.05	112.85	118.30
2	B	211	TYR	O-C-N	-6.01	113.09	122.70
2	D	138	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	G	9	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	G	29	HIS	N-CA-CB	6.00	121.41	110.60
1	C	52	ALA	O-C-N	-6.00	113.00	123.20
2	D	88	ASN	CB-CA-C	5.99	122.38	110.40
1	G	101	TYR	CA-C-N	5.99	130.38	117.20
2	H	128	ASN	CB-CA-C	-5.96	98.49	110.40
2	F	207	ASP	CB-CG-OD1	5.95	123.65	118.30
2	B	48	ASP	CB-CG-OD1	5.92	123.63	118.30
2	B	49	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	100	LEU	CB-CG-CD2	5.91	121.05	111.00
2	F	148	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	H	108	CYS	CA-CB-SG	5.89	124.59	114.00
1	A	32	MET	CG-SD-CE	-5.88	90.80	100.20
1	G	59	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	E	50	TYR	CA-CB-CG	5.86	124.53	113.40
2	D	69	LEU	CB-CG-CD1	5.84	120.93	111.00
1	E	80	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	E	117	LEU	CA-CB-CG	5.78	128.60	115.30
2	H	55	ASP	CB-CG-OD1	5.72	123.45	118.30
2	H	7	MET	CG-SD-CE	5.68	109.29	100.20
1	E	96	GLY	N-CA-C	-5.68	98.91	113.10
1	A	57	LYS	CD-CE-NZ	5.67	124.74	111.70
2	B	157	LEU	CB-CA-C	-5.67	99.44	110.20
1	G	101	TYR	CB-CG-CD1	-5.64	117.61	121.00
1	A	44	ARG	NE-CZ-NH1	-5.63	117.49	120.30
2	D	171	LEU	CB-CG-CD1	5.63	120.57	111.00
2	H	112	GLY	N-CA-C	5.62	127.16	113.10
2	D	63	LYS	CD-CE-NZ	-5.59	98.83	111.70
1	E	45	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	89	VAL	CB-CA-C	-5.55	100.85	111.40
2	B	196	TYR	CB-CG-CD2	5.55	124.33	121.00
2	D	60	ASN	N-CA-C	5.54	125.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	71	SER	N-CA-CB	5.54	118.81	110.50
1	C	75	PHE	CB-CA-C	-5.54	99.33	110.40
1	G	46	ILE	CG1-CB-CG2	-5.54	99.22	111.40
2	B	76	LYS	CD-CE-NZ	-5.53	98.97	111.70
2	B	166	ILE	CG1-CB-CG2	-5.53	99.23	111.40
2	H	172	TYR	N-CA-C	-5.51	96.13	111.00
1	C	55	THR	N-CA-CB	5.50	120.75	110.30
1	A	77	LEU	O-C-N	5.50	131.49	122.70
2	H	11	LEU	CB-CA-C	-5.48	99.78	110.20
2	H	64	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	C	23	CYS	CB-CA-C	5.47	121.34	110.40
1	E	80	GLU	CB-CA-C	5.47	121.34	110.40
1	E	97	GLY	N-CA-C	5.46	126.74	113.10
2	B	69	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	G	9	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	66	LYS	CD-CE-NZ	-5.43	99.22	111.70
2	B	198	MET	CB-CG-SD	5.42	128.66	112.40
2	H	126	LEU	CB-CG-CD1	-5.42	101.79	111.00
2	D	91	VAL	CA-C-N	-5.42	105.28	117.20
2	F	132	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	B	63	LYS	CD-CE-NZ	5.41	124.13	111.70
1	A	22	SER	CB-CA-C	-5.40	99.84	110.10
2	B	230	VAL	N-CA-C	-5.37	96.50	111.00
1	G	50	TYR	CB-CG-CD2	5.36	124.22	121.00
2	D	55	ASP	CB-CG-OD1	5.36	123.12	118.30
2	F	7	MET	CA-CB-CG	5.35	122.39	113.30
2	F	120	HIS	N-CA-C	5.33	125.38	111.00
2	B	198	MET	CA-CB-CG	-5.32	104.25	113.30
2	B	92	ASN	N-CA-CB	5.32	120.17	110.60
1	E	53	GLY	N-CA-C	5.31	126.39	113.10
1	G	30	ASN	CB-CA-C	-5.31	99.78	110.40
2	F	172	TYR	N-CA-C	-5.30	96.69	111.00
2	D	58	LEU	CB-CG-CD1	-5.28	102.02	111.00
2	F	132	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	D	225	SER	N-CA-CB	-5.25	102.62	110.50
1	A	31	ASN	CB-CA-C	-5.24	99.92	110.40
1	G	101	TYR	C-N-CA	5.24	134.79	121.70
1	G	69	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	D	104	GLY	N-CA-C	-5.22	100.06	113.10
1	A	77	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	75	PHE	CB-CG-CD2	5.17	124.42	120.80
1	C	54	SER	N-CA-CB	5.17	118.26	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	TYR	N-CA-CB	-5.17	101.30	110.60
2	B	132	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	G	99	THR	CB-CA-C	-5.14	97.71	111.60
2	B	62	ASP	CB-CG-OD1	-5.14	113.68	118.30
2	D	73	LEU	CA-CB-CG	5.13	127.11	115.30
2	B	224	LYS	CA-CB-CG	5.13	124.69	113.40
1	C	57	LYS	CB-CA-C	-5.13	100.14	110.40
2	F	169	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	G	50	TYR	N-CA-C	5.12	124.83	111.00
2	H	165	LEU	CB-CG-CD1	5.12	119.70	111.00
2	D	214	MET	CB-CG-SD	-5.11	97.06	112.40
2	B	162	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	52	ALA	CB-CA-C	5.10	117.75	110.10
2	D	73	LEU	N-CA-C	-5.10	97.23	111.00
2	B	196	TYR	CB-CA-C	-5.10	100.21	110.40
1	G	59	ASP	OD1-CG-OD2	5.09	132.98	123.30
2	F	33	VAL	CB-CA-C	-5.09	101.73	111.40
2	D	107	THR	CA-CB-CG2	5.09	119.52	112.40
2	F	33	VAL	CG1-CB-CG2	5.08	119.03	110.90
2	B	229	GLU	OE1-CD-OE2	5.08	129.39	123.30
2	H	207	ASP	CB-CG-OD2	-5.08	113.73	118.30
2	B	167	ASN	N-CA-C	-5.07	97.32	111.00
2	F	162	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	F	158	ASP	CB-CG-OD2	5.05	122.84	118.30
1	C	85	SER	N-CA-CB	-5.04	102.94	110.50
1	A	59	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	55	THR	CB-CA-C	-5.03	98.01	111.60
1	A	93	ALA	N-CA-C	-5.03	97.42	111.00
1	A	66	LYS	CG-CD-CE	-5.02	96.83	111.90
2	D	79	ASP	CB-CG-OD1	5.01	122.81	118.30
2	H	226	VAL	N-CA-C	5.01	124.52	111.00
2	B	108	CYS	CA-CB-SG	5.00	123.00	114.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	828	0	786	79	1
1	C	828	0	786	79	1
1	E	828	0	786	60	0
1	G	828	0	787	66	0
2	B	1904	0	1847	125	0
2	D	1913	0	1852	121	0
2	F	1906	0	1839	135	0
2	H	1922	0	1853	155	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	803	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 37.

All (803) 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:CB	1:A:26:THR:CG2	1.76	1.60
2:B:27:LEU:CG	2:B:27:LEU:CD1	1.86	1.53
1:E:80:GLU:CG	1:E:80:GLU:CD	1.75	1.51
1:G:101:TYR:C	1:G:108:PHE:N	1.74	1.41
1:A:32:MET:SD	1:A:32:MET:CE	2.08	1.40
1:E:63:GLY:C	1:E:65:TYR:N	1.76	1.38
1:C:63:GLY:C	1:C:65:TYR:N	1.80	1.33
1:E:101:TYR:C	1:E:108:PHE:N	1.83	1.31
1:A:101:TYR:C	1:A:108:PHE:N	1.87	1.26
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: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:HE3	2:D:56:LYS:HA	1.17	1.11
1:A:63:GLY:C	1:A:65:TYR:N	2.04	1.10
2:D:13:LYS:HB3	2:D:180:GLU:OE1	1.49	1.10
1:C:87:THR:HG23	1:C:115:SER:HA	1.32	1.10
1:A:87:THR:HG23	1:A:115:SER:HA	1.12	1.07
2:D:162:ARG:HG3	2:D:162:ARG:HH11	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:CA	2:D:56:LYS:HE3	1.92	0.98
2:D:162:ARG:NH1	2:D:162:ARG:HG3	1.64	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:O	1:E:4:VAL:HG12	1.66	0.94
1:A:24:GLN:OE1	1:A:74:GLN:NE2	1.99	0.94
2:F:37:LYS:HB2	2:F:116:HIS:CD2	2.03	0.93
2:B:190:ASN:HD22	2:B:190:ASN:C	1.70	0.93
1:E:32:MET:HE1	1:E:75:PHE:HB3	1.51	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
1:E:32:MET:CE	1:E:75:PHE:HB3	1.98	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:G:18:LYS:NZ	1:G:18:LYS:HB3	1.83	0.92
2:F:35:ALA:HB3	2:F:84:VAL:CG2	1.99	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:B:24:MET:HE1	2:B:28:TYR:HE1	1.33	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:HH11	2:B:138:ARG:HG3	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:E:32:MET:HE2	1:E:75:PHE:CB	2.00	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
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:O	1:C:37:GLN:HG3	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
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
1:C:88:SER:OG	1:C:89:VAL:N	2.05	0.85
2:F:49:LEU:HD11	2:F:78:LYS:HA	1.59	0.85
1:E:32:MET:CE	1:E:75:PHE:CB	2.55	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
2:F:195:TRP:O	2:F:196:TYR:CD2	2.29	0.84
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
2:D:158:ASP:CG	2:D:162:ARG:HH12	1.81	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
2:D:58:LEU:CD1	3:D:250:HOH:O	2.25	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:162:ARG:HD3	2:D:198:MET:CE	2.11	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:D:162:ARG:HD3	2:D:198:MET:HE2	1.63	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: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:HD1	1:C:108:PHE:N	1.80	0.79
2:H:194:PHE:CD1	2:H:194:PHE:O	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:B:24:MET:HE1	2:B:28:TYR:CE1	2.20	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:D:143:PHE:HE2	2:D:145:VAL:CG1	1.99	0.75
2:B:224:LYS:HB3	3:B:279:HOH:O	1.86	0.74
2:B:190:ASN:ND2	2:B:190:ASN:O	2.21	0.74
2:D:234:THR:O	2:D:235:LYS:NZ	2.18	0.74
2:H:42:ASP:OD1	2:H:43:LYS:N	2.21	0.74
2:D:226:VAL:O	2:D:227:LYS:HD3	1.88	0.74
1:C:54:SER:O	1:C:55:THR:HG22	1.87	0.73
2:H:86:GLY:HA2	2:H:155:GLN:OE1	1.86	0.73
2:D:33:VAL:O	2:D:85:TYR:HA	1.88	0.73
1:C:87:THR:CG2	1:C:115:SER:HA	2.17	0.73
2:D:55:ASP:OD1	2:D:60:ASN:HB2	1.87	0.73
2:F:83:ASP:HB2	2:F:114:THR:OG1	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:SER:HB2	3:B:254:HOH:O	1.88	0.72
2:D:127:GLN:HE21	2:D:224:LYS:HB3	1.54	0.72
2:D:68:LEU:HD11	2:D:113:ILE:HD12	1.71	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:B:190:ASN:ND2	2:B:190:ASN:C	2.42	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
1:E:32:MET:HE2	1:E:75:PHE:HB2	1.73	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
1:E:101:TYR:C	1:E:108:PHE:CA	2.61	0.70
2:F:11:LEU:HD11	2:F:183:TYR:CD2	2.27	0.70
2:B:184:ILE:HG13	2:B:230:VAL:HG22	1.74	0.70
1:C:83:THR:HG23	1:C:85:SER:HB2	1.74	0.69
2:H:31:HIS:CE1	2:H:88:ASN:ND2	2.61	0.69
2:D:184:ILE:HG23	2:D:184:ILE:O	1.92	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:130:LEU:HD12	2:H:131:VAL:N	2.07	0.69
2:H:88:ASN:HD22	2:H:88:ASN:H	1.40	0.69
2:B:223:SER:O	2:B:225:SER:N	2.26	0.69
2:B:20:THR:O	2:B:23:ASN:HB2	1.93	0.69
1:C:9:ARG:NH1	1:C:9:ARG:HB3	2.08	0.68
1:G:66:LYS:HB3	2:H:174:PHE:CE2	2.28	0.68
2:D:24:MET:HE2	2:D:28:TYR:HE1	1.58	0.68
1:E:24:GLN:HE22	1:E:74:GLN:CD	1.97	0.68
1:G:35:TYR:HA	1:G:44:ARG:O	1.93	0.68
2:F:237:GLY:OXT	1:G:113:ARG:HG2	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
2:H:86:GLY:CA	2:H:155:GLN:OE1	2.41	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:D:112:GLY:HA2	2:D:153:THR:HG21	1.76	0.68
1:E:74:GLN:O	1:E:74:GLN:HG3	1.88	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:THR:HG23	2:H:233:THR:HB	1.76	0.67
2:F:27:LEU:HA	2:F:31:HIS:HD2	1.60	0.67
1:G:57:LYS:NZ	2:H:18:THR:O	2.26	0.67
1:G:59:ASP:O	1:G:61:PRO:HD3	1.95	0.67
2:B:6:PRO:HD3	2:B:195:TRP:CE2	2.30	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
2:B:107:THR:OG1	2:B:108:CYS:N	2.24	0.66
1:A:68:SER:O	1:A:70:PRO:HD3	1.95	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:O	2:H:233:THR:HG22	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: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
2:B:19:GLY:H	2:B:204:ASP:HA	1.60	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:F:37:LYS:HB2	2:F:116:HIS:HD2	1.57	0.64
2:B:132:ARG:HD2	2:B:227:LYS:HE2	1.78	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
1:C:101:TYR:C	1:C:108:PHE:N	2.52	0.63
2:D:47:HIS:HE1	2:D:67:GLU:OE1	1.81	0.63
2:H:155:GLN:HE21	2:H:215:TYR:CB	2.05	0.63
1:E:44:ARG:CG	1:E:44:ARG:HH21	2.11	0.63
2:B:171:LEU:HD21	2:B:198:MET:CE	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:THR:HG21	2:H:152:VAL:CG2	2.28	0.63
2:F:95:PHE:CZ	2:F:106:LYS:HD3	2.34	0.63
2:D:95:PHE:CZ	2:D:106:LYS:HB2	2.34	0.63
1:C:74:GLN:HG3	1:C:75:PHE:N	2.06	0.63
2:D:121:PHE:CE1	2:D:127:GLN:HB2	2.34	0.63
2:H:140:THR:C	2:H:141:ILE:HG23	2.19	0.63
2:H:80:GLU:HB3	2:H:82:VAL:HG13	1.80	0.63
2:F:45:LEU:HD13	2:F:47:HIS:CE1	2.31	0.63
1:C:25:GLN:CG	1:C:25:GLN:O	2.46	0.63
1:G:14:VAL:O	1:G:15:THR:C	2.35	0.62
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:B:87:SER:O	2:B:212:LEU:HD22	1.99	0.62
2:F:31:HIS:O	2:F:32:TYR:HB3	1.98	0.62
2:D:5:ASP:OD1	2:D:185:LYS:HE3	1.98	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
1:G:66:LYS:HE3	1:G:80:GLU:HG2	1.82	0.62
2:F:27:LEU:HA	2:F:31:HIS:CD2	2.35	0.62
2:B:52:ASN:OD1	2:B:63:LYS:HD3	1.99	0.62
1:A:87:THR:HG22	1:A:115:SER:HA	1.77	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:24:MET:CE	2:B:28:TYR:HE1	2.10	0.61
2:D:24:MET:HE2	2:D:28:TYR:CE1	2.35	0.61
2:B:123:ASN:HB2	3:B:245:HOH:O	2.00	0.61
2:H:194:PHE:HD1	2:H:194:PHE:O	1.81	0.61
2:B:25:LYS:HG2	3:B:271:HOH:O	1.99	0.61
1:E:44:ARG:HB2	1:E:60:ILE:CD1	2.30	0.61
2:B:175:ASN:HB3	3:B:268:HOH:O	2.00	0.61
2:F:80:GLU:HA	2:F:80:GLU:OE2	2.00	0.61
2:H:222:ASP:O	2:H:226:VAL:CG1	2.49	0.61
1:E:14:VAL:O	1:E:16:GLY:N	2.34	0.61
2:F:37:LYS:O	2:F:37:LYS:HG2	2.01	0.61
1:G:87:THR:CG2	1:G:115:SER:HA	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:ASP:HB3	2:F:58:LEU:O	2.01	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: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:F:35:ALA:CB	2:F:84:VAL:HG23	2.31	0.60
2:H:27:LEU:HD23	2:H:27:LEU:N	2.15	0.60
1:C:37:GLN:CG	1:C:37:GLN:O	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
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:H:40:SER:CB	2:H:49:LEU:HD22	2.32	0.59
2:F:136:ASN:OD1	2:F:233:THR:HA	2.03	0.59
1:E:101:TYR:O	1:E:108:PHE:HA	2.03	0.59
1:A:52:ALA:HA	1:A:69:ARG:HG2	1.84	0.59
2:F:116:HIS:ND1	2:F:116:HIS:C	2.56	0.59
2:B:138:ARG:NH1	2:B:138:ARG:CG	2.57	0.59
1:A:9:ARG:NH2	1:A:111:GLY:O	2.35	0.58
2:H:39:LYS:CG	2:H:80:GLU:O	2.50	0.58
2:B:86:GLY:HA3	2:B:109:MET:HE3	1.84	0.58
2:H:45:LEU:HD23	2:H:47:HIS:CE1	2.38	0.58
1:A:32:MET:CE	1:A:32:MET:CG	2.82	0.58
1:A:27:ASN:HB3	1:A:29:HIS:CE1	2.37	0.58
2:F:216:ASN:ND2	2:F:217:ASP:N	2.51	0.58
2:D:6:PRO:HG3	2:D:195:TRP:CE2	2.39	0.58
2:H:6:PRO:HD3	2:H:195:TRP:CE2	2.39	0.58
2:B:155:GLN:NE2	2:B:215:TYR:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:MET:CE	2:B:28:TYR:CE1	2.84	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:H:171:LEU:HD21	2:H:198:MET:CE	2.33	0.58
1:E:63:GLY:C	1:E:65:TYR:CA	2.70	0.58
2:D:162:ARG:HD3	2:D:198:MET:HE3	1.85	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:C:101:TYR:C	1:C:108:PHE:HA	2.25	0.57
1:A:24:GLN:HA	1:A:73:GLU:O	2.04	0.57
2:H:39:LYS:HG3	2:H:80: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: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: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
1:C:36:ARG:O	1:C:36:ARG:HG3	2.04	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:H:77:TYR:C	2:H:79:ASP:H	2.08	0.57
2:F:110:TYR:HE1	2:F:209:SER:O	1.86	0.57
1:C:41:HIS:O	1:C:42:GLY:C	2.40	0.57
2:B:101:LYS:C	2:B:103:THR:H	2.08	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:87:THR:HG23	1:E:115:SER:HA	1.87	0.56
2:F:82:VAL:HG12	2:F:114:THR:C	2.25	0.56
1:E:44:ARG:HB3	1:E:60:ILE:HD13	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:38:ASP:OD1	1:E:88:SER:OG	2.20	0.56
2:H:155:GLN:HG3	2:H:215:TYR:CD1	2.40	0.56
1:G:18:LYS:HB3	1:G:18:LYS:HZ2	1.68	0.56
2:D:55:ASP:HA	2:D:61:TYR:CE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:LEU:CD2	2:H:148:ASP:HB3	2.34	0.56
1:G:37:GLN:O	1:G:37:GLN:HG2	2.03	0.56
2:H:225:SER:OG	2:H:226:VAL:N	2.33	0.56
2:B:156:GLU:O	2:B:160:LYS:HG3	2.06	0.56
1:G:9:ARG:HD3	1:G:9:ARG:O	2.05	0.56
2:B:27:LEU:CD1	2:B:27:LEU:CB	2.73	0.56
1:A:70:PRO:HD2	1:A:74:GLN:HB3	1.88	0.56
1:E:31:ASN:O	1:E:32:MET:HG2	2.06	0.56
1:G:15:THR:OG1	1:G:84:PRO:HD3	2.05	0.56
2:F:35:ALA:HB3	2:F:84:VAL:HG22	1.83	0.56
2:F:71:GLU:HG2	2:F:71:GLU:O	2.06	0.56
2:D:143:PHE:CE2	2:D:145:VAL:CG1	2.86	0.56
2:B:153:THR:HA	2:B:220:THR:HA	1.88	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: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
2:D:14:SER:C	2:D:16:GLU:H	2.10	0.55
1:G:72:GLN:HA	1:G:72:GLN:OE1	2.06	0.55
1:G:18:LYS:HB3	1:G:18:LYS:HZ3	1.69	0.55
2:H:171:LEU:HD21	2:H:198:MET:HE2	1.88	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
1:C:101:TYR:O	1:C:108:PHE:C	2.44	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:H:171:LEU:O	2:H:177:SER:OG	2.21	0.55
2:F:194:PHE:HD2	2:F:194:PHE:H	1.53	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:228:ILE:HG22	2:D:229:GLU:N	2.22	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
1:E:108:PHE:N	1:E:108:PHE:CD1	2.75	0.55
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:13:LYS:CB	2:D:180:GLU:OE1	2.38	0.55
2:D:6:PRO:HG3	2:D:195:TRP:CZ2	2.42	0.55
2:H:89:TYR:CZ	2:H:209:SER:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:197:ASP:OD1	2:F:198:MET:N	2.39	0.54
2:B:88:ASN:HD22	2:B:88:ASN:H	1.54	0.54
2:H:61:TYR:CG	2:H:107:THR:HG22	2.42	0.54
2:B:7:MET:O	2:B:9:ASP:N	2.41	0.54
2:F:236:ASN:HD22	2:F:236:ASN:N	2.05	0.54
2:F:44:PHE:HD2	2:F:96:SER:HG	1.50	0.54
2:H:155:GLN:HG3	2:H:215:TYR:CD2	2.42	0.54
1:A:38:ASP:OD1	1:A:44:ARG:NH1	2.40	0.54
2:F:53:ILE:HD11	2:F:84:VAL:HG21	1.87	0.54
2:B:184:ILE:HG23	2:B:184:ILE:O	2.07	0.54
1:C:74:GLN:HE21	1:C:76:SER:HB3	1.71	0.54
1:A:88:SER:OG	1:A:89:VAL:N	2.40	0.54
1:C:68:SER:O	1:C:70:PRO:HD3	2.07	0.54
1:E:44:ARG:CB	1:E:60:ILE:CD1	2.86	0.54
2:B:95:PHE:CZ	2:B:106:LYS:HG2	2.43	0.54
2:H:151:SER:HA	2:H:221:VAL:O	2.08	0.54
2:H:102:VAL:HG12	2:H:102:VAL:O	2.07	0.54
2:B:170:ASN:O	2:B:171:LEU:C	2.45	0.54
2:B:217:ASP:C	2:B:217:ASP:OD1	2.46	0.54
2:H:129:VAL:HG12	2:H:130:LEU:N	2.22	0.54
1:C:9:ARG:CZ	1:C:9:ARG:HB3	2.37	0.54
2:F:120:HIS:O	2:F:150:LYS:NZ	2.41	0.54
2:B:47:HIS:NE2	2:B:67:GLU:OE1	2.32	0.54
2:H:99:ASP:HB3	2:H:102:VAL:HA	1.89	0.53
2:F:19:GLY:CA	3:F:238:HOH:O	2.54	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
1:A:4:VAL:HG21	1:A:94:SER:HB3	1.89	0.53
2:H:147:THR:CG2	2:H:152:VAL:HG21	2.39	0.53
2:D:162:ARG:CD	2:D:198:MET:HE3	2.39	0.53
2:H:140:THR:O	2:H:141:ILE:CG2	2.57	0.53
1:E:33:TYR:N	1:E:33:TYR:CD1	2.76	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
1:G:17:GLU:HG3	1:G:18:LYS:H	1.70	0.53
2:D:76:LYS:O	2:D:76:LYS:HG3	2.09	0.53
2:F:164:PHE:O	2:F:168:LYS:HD3	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:55:ASP:OD2	2:B:56:LYS:N	2.43	0.52
2:B:5:ASP:OD1	2:B:185:LYS:NZ	2.34	0.52
2:F:180:GLU:OE1	2:F:180:GLU:HA	2.08	0.52
2:F:45:LEU:CD1	2:F:47:HIS:HE1	2.16	0.52
2:H:149:LYS:O	2:H:223:SER:OG	2.24	0.52
2:H:162:ARG:O	2:H:166:ILE:HG13	2.10	0.52
2:F:62:ASP:HB2	3:F:261:HOH:O	2.09	0.52
1:C:9:ARG:CG	1:C:9:ARG:HH11	2.22	0.52
1:G:80:GLU:O	1:G:81:SER:CB	2.55	0.52
1:E:14:VAL:O	1:E:15:THR:C	2.47	0.52
2:H:13:LYS:HD3	2:H:180:GLU:OE1	2.10	0.52
2:F:149:LYS:HE2	2:F:156:GLU:OE2	2.09	0.52
2:D:194:PHE:HZ	2:D:221:VAL:HG11	1.74	0.52
2:D:76:LYS:O	2:D:76:LYS:CG	2.56	0.52
2:B:33:VAL:CG1	2:B:34:SER:H	2.16	0.52
2:H:184:ILE:HG13	2:H:230:VAL:HG22	1.92	0.52
2:F:157:LEU:HD12	2:F:186:PHE:HE2	1.75	0.52
2:B:152:VAL:HG13	2:B:152:VAL:O	2.09	0.52
2:F:152:VAL:HG11	2:F:157:LEU:HD21	1.91	0.52
1:E:101:TYR:O	1:E:108:PHE:CA	2.58	0.52
1:E:32:MET:HE2	1:E:75:PHE:CG	2.44	0.52
2:D:54:SER:O	2:D:55:ASP:C	2.48	0.52
1:G:66:LYS:CB	2:H:174:PHE:CE2	2.92	0.52
1:G:4:VAL:HG12	1:G:109:GLY:CA	2.40	0.52
2:B:39:LYS:HD2	2:B:79:ASP:O	2.10	0.52
1:C:69:ARG:CG	1:C:69:ARG:HH21	2.23	0.52
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:47:HIS:H	2:D:47:HIS:CD2	2.28	0.51
2:D:20:THR:HG21	2:D:174:PHE:CZ	2.46	0.51
2:D:121:PHE:CZ	2:D:127:GLN:HB2	2.45	0.51
2:D:159:ILE:CG2	2:D:159:ILE:O	2.54	0.51
2:B:200:PRO:O	2:B:201:ALA:C	2.47	0.51
2:D:136:ASN:HD21	2:D:234:THR:H	1.58	0.51
2:B:224:LYS:O	2:B:225:SER:HB3	2.11	0.51
2:B:169:LYS:HB3	2:B:179:TYR:OH	2.09	0.51
1:A:38:ASP:O	1:A:41:HIS:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:29:ASP:O	2:B:30:ASP:C	2.47	0.51
2:F:69:LEU:H	2:F:73:LEU:HD23	1.76	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
2:B:213:MET:O	2:B:216:ASN:HB2	2.11	0.51
1:C:25:GLN:OE1	1:C:29:HIS:N	2.41	0.51
1:G:31:ASN:N	1:G:31:ASN:HD22	2.08	0.51
2:F:90:TYR:O	2:F:92:ASN:N	2.44	0.51
1:A:41:HIS:C	1:A:42:GLY:O	2.49	0.51
2:D:42:ASP:CG	2:D:43:LYS:H	2.14	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
1:E:4:VAL:CG1	1:E:4:VAL:O	2.40	0.50
2:B:33:VAL:CG1	2:B:34:SER:N	2.71	0.50
2:H:51:TYR:HB2	2:H:53:ILE:CD1	2.39	0.50
2:F:205:LYS:N	2:F:205:LYS:HD3	2.25	0.50
2:F:33:VAL:N	2:F:86:GLY:O	2.41	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
2:F:186:PHE:C	2:F:187:ILE:HG13	2.32	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:C:33:TYR:CD1	1:C:33:TYR:N	2.79	0.50
1:A:33:TYR:HB2	1:A:93:ALA:HB3	1.94	0.50
1:E:87:THR:CG2	1:E:115:SER:HA	2.42	0.50
2:H:27:LEU:HA	2:H:31:HIS:HD2	1.75	0.50
1:G:55:THR:HB	3:G:121:HOH:O	2.11	0.50
2:B:19:GLY:N	2:B:204:ASP:HA	2.26	0.50
2:H:13:LYS:HB3	2:H:180:GLU:OE1	2.12	0.50
2:F:204:ASP:OD1	2:F:205:LYS:HE3	2.10	0.50
1:E:28:ASN:CG	1:E:28:ASN:O	2.50	0.50
2:F:194:PHE:N	3:F:244:HOH:O	2.43	0.50
1:G:12:VAL:HG11	1:G:117:LEU:CD1	2.42	0.49
2:F:68:LEU:HD11	2:F:113:ILE:CD1	2.42	0.49
2:H:27:LEU:HA	2:H:31:HIS:CD2	2.48	0.49
2:D:134:TYR:CE2	2:D:139:ASN:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HG2	1:A:46:ILE:HD11	1.94	0.49
1:A:38:ASP:O	1:A:39:THR:C	2.50	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: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:H:39:LYS:HG2	2:H:80:GLU:O	2.13	0.49
1:E:44:ARG:HB2	1:E:60:ILE:HD12	1.93	0.49
1:E:14:VAL:H	1:E:17:GLU:HG2	1.77	0.49
1:G:51:GLY:HA3	2:H:91:VAL:HG22	1.94	0.49
1:E:79:LEU:O	1:E:80:GLU:C	2.51	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:B:171:LEU:HD21	2:B:198:MET:HE2	1.94	0.49
2:D:135:GLU:HA	2:D:232:LEU:O	2.13	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:CB	1:A:9:ARG:NH1	2.67	0.49
2:F:6:PRO:HG3	2:F:195:TRP:CE2	2.48	0.49
1:E:32:MET:C	1:E:33:TYR:CD1	2.86	0.49
2:H:77:TYR:C	2:H:79:ASP:N	2.66	0.49
2:F:187:ILE:HA	2:F:193:THR:HG22	1.95	0.49
2:H:194:PHE:CD1	2:H:194:PHE:C	2.86	0.48
1:A:54:SER:HA	2:B:23:ASN:OD1	2.13	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
2:H:169:LYS:O	2:H:170:ASN:HB2	2.13	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:94:TYR:O	2:D:95:PHE:HB3	2.12	0.48
1:C:24:GLN:N	1:C:24:GLN:CD	2.67	0.48
2:F:165:LEU:O	2:F:166:ILE:O	2.31	0.48
2:D:102:VAL:O	2:D:102:VAL:HG23	2.14	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:27:LEU:CD1	2:B:27:LEU:CD2	2.88	0.48
2:B:8:PRO:O	2:B:13:LYS:CE	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:LEU:HG	1:G:78:ILE:N	2.29	0.48
2:F:119:ASN:O	2:F:150:LYS:HG3	2.13	0.48
2:B:21:MET:O	2:B:24:MET:HB3	2.14	0.47
1:C:43:LEU:HD12	1:C:43:LEU:HA	1.56	0.47
1:C:67:ALA:O	1:C:68:SER:CB	2.60	0.47
2:B:139:ASN:O	2:B:139:ASN:ND2	2.47	0.47
2:H:33:VAL:O	2:H:85:TYR:HA	2.13	0.47
1:E:32:MET:HE2	1:E:75:PHE:CD2	2.50	0.47
2:B:188:GLU:HG3	2:B:192:ASN:HB3	1.96	0.47
2:B:24:MET:O	2:B:25:LYS:C	2.52	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
1:G:18:LYS:CB	1:G:18:LYS:NZ	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
2:B:12:HIS:HB2	2:B:197:ASP:OD2	2.15	0.47
1:A:26:THR:CG2	1:A:26:THR:CA	2.80	0.47
1:G:114:LEU:HD21	1:G:116:VAL:CG2	2.44	0.47
2:F:45:LEU:CD1	2:F:47:HIS:CE1	2.95	0.47
1:G:21:LEU:O	1:G:76:SER:HB2	2.14	0.47
2:D:49:LEU:HD21	2:D:78:LYS:CB	2.42	0.47
2:H:49:LEU:CD2	2:H:78:LYS:HA	2.44	0.47
2:D:68:LEU:H	2:D:68:LEU:HD22	1.77	0.47
2:B:213:MET:HE3	3:B:244:HOH:O	2.13	0.47
2:F:115:LYS:CD	2:F:116:HIS:N	2.76	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:B:179:TYR:HB3	2:B:233:THR:O	2.15	0.47
2:H:184:ILE:O	2:H:195:TRP:HA	2.15	0.47
2:H:37:LYS:HE2	2:H:116:HIS:CE1	2.50	0.47
2:D:155:GLN:O	2:D:156:GLU:C	2.53	0.47
1:C:44:ARG:HE	1:C:44:ARG:HB2	1.58	0.47
1:E:93:ALA:HB1	1:E:100:LEU:HD22	1.96	0.46
1:A:38:ASP:HB2	1:A:44:ARG:NH1	2.30	0.46
1:G:83:THR:C	1:G:116:VAL:HG11	2.36	0.46
1:C:30:ASN:O	1:C:69:ARG:NH1	2.42	0.46
2:B:113:ILE:HG21	2:B:113:ILE:HD13	1.56	0.46
2:B:136:ASN:O	2:B:138:ARG:NH1	2.48	0.46
2:H:227:LYS:HZ2	2:H:227:LYS:HA	1.79	0.46
1:C:25:GLN:O	1:C:25:GLN:HG3	2.09	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:HA	1:E:115:SER:O	2.14	0.46
2:B:13:LYS:CB	2:B:180:GLU:OE1	2.61	0.46
2:F:188:GLU:HB2	2:F:192:ASN:HB3	1.96	0.46
2:H:82:VAL:HG11	2:H:113:ILE:CG2	2.46	0.46
2:F:193:THR:C	3:F:244:HOH:O	2.53	0.46
2:D:182:GLY:HA2	2:D:231:HIS:O	2.15	0.46
2:H:218:ASN:HA	3:H:242:HOH:O	2.14	0.46
2:H:132:ARG:HG2	2:H:142:SER:HB3	1.96	0.46
2:D:42:ASP:OD2	2:D:43:LYS:N	2.48	0.46
1:A:45:LEU:HD21	1:A:48:TYR:HD1	1.80	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
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
1:C:33:TYR:HB3	1:C:45:LEU:CD1	2.46	0.46
2:H:61:TYR:CD2	2:H:107:THR:HG21	2.51	0.46
2:D:46:ALA:HB1	2:D:71:GLU:HB2	1.97	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:D:12:HIS:O	2:D:181:THR:HG22	2.15	0.46
1:G:87:THR:HG22	1:G:114:LEU:O	2.12	0.46
2:H:128:ASN:HD22	2:H:144:GLU:CD	2.19	0.46
1:C:3:ALA:HA	1:C:26:THR:HB	1.98	0.46
1:C:116:VAL:O	1:C:116:VAL:HG12	2.16	0.46
2:F:41:VAL:O	2:F:42:ASP:CB	2.64	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
1:A:23:CYS:SG	1:A:32:MET:CE	3.04	0.45
1:C:65:TYR:CD1	1:C:77:LEU:HD11	2.51	0.45
2:B:171:LEU:HD21	2:B:198:MET:HE3	1.99	0.45
1:A:117:LEU:HA	1:A:117:LEU:HD23	1.77	0.45
2:B:100:GLY:O	2:B:102:VAL:N	2.49	0.45
2:H:99:ASP:HB3	2:H:102:VAL:CA	2.47	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:B:31:HIS:HB2	3:B:241:HOH:O	2.17	0.45
1:E:36:ARG:HG2	1:E:60:ILE:HD11	1.99	0.45
2:D:206:PHE:CE2	2:D:208:GLN:HG3	2.52	0.45
2:D:126:LEU:HD22	2:D:147:THR:O	2.17	0.45
2:F:49:LEU:HD22	2:F:74:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:LEU:O	2:H:213:MET:C	2.55	0.45
2:B:70:ASN:HB2	2:B:71:GLU:H	1.42	0.45
1:C:28:ASN:HA	1:C:72:GLN:HG2	1.99	0.45
1:E:11:LYS:HE3	1:E:19:VAL:HG13	1.99	0.45
2:H:55:ASP:HB2	2:H:61:TYR:CE2	2.51	0.45
2:F:206:PHE:HB2	3:F:240:HOH:O	2.17	0.45
1:E:71:SER:OG	1:E:74:GLN:HB3	2.17	0.45
2:H:67:GLU:HG2	2:H:110:TYR:CE2	2.52	0.45
1:A:46:ILE:CD1	1:A:77:LEU:HD21	2.46	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
2:H:140:THR:C	2:H:141:ILE:CG2	2.85	0.45
1:A:46:ILE:HD12	1:A:77:LEU:HD21	1.99	0.45
1:C:63:GLY:CA	1:C:65:TYR:N	2.73	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:N	2:F:90:TYR:CD1	2.85	0.44
2:D:128:ASN:HD22	2:D:144:GLU:CD	2.21	0.44
1:E:32:MET:HE1	1:E:75:PHE:CB	2.29	0.44
2:F:110:TYR:HD1	2:F:212:LEU:C	2.21	0.44
2:F:204:ASP:C	2:F:205:LYS:HD3	2.37	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
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:HD23	2:D:49:LEU:HA	1.55	0.44
1:C:77:LEU:HD12	1:C:78:ILE:H	1.83	0.44
1:E:44:ARG:NH2	1:E:44:ARG:HG3	2.25	0.44
2:H:67:GLU:HG3	2:H:67:GLU:O	2.18	0.44
2:B:31:HIS:HA	2:B:57:LYS:HE2	1.99	0.44
1:A:32:MET:HE2	1:A:32:MET:HB3	2.00	0.44
2:D:5:ASP:HA	2:D:6:PRO:HD3	1.75	0.44
2:F:55:ASP:OD2	2:F:60:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:31:ASN:ND2	1:C:50:TYR:CD1	2.86	0.44
2:F:20:THR:HG22	2:F:20:THR:O	2.18	0.44
2:H:236:ASN:ND2	2:H:236:ASN:N	2.66	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:D:228:ILE:CG2	2:D:229:GLU:N	2.81	0.44
2:H:150:LYS:O	2:H:223:SER:N	2.37	0.44
2:F:184:ILE:O	2:F:184:ILE:HG23	2.16	0.44
1:G:28:ASN:O	1:G:28:ASN:CG	2.56	0.44
2:F:3:GLN:HB2	2:F:3:GLN:HE21	1.57	0.44
2:H:202:PRO:HG3	3:H:244:HOH:O	2.17	0.44
2:B:18:THR:N	2:B:203:GLY:O	2.32	0.44
1:A:69:ARG:HH21	1:A:69:ARG:HD3	1.61	0.43
2:F:89:TYR:C	2:F:89:TYR:CD2	2.91	0.43
2:H:207:ASP:HB3	2:H:210:LYS:HB3	2.00	0.43
1:C:66:LYS:HG3	1:C:66:LYS:HZ3	1.48	0.43
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.79	0.43
2:H:227:LYS:HZ2	2:H:228:ILE:H	1.66	0.43
2:B:65:LYS:HD3	2:B:95:PHE:HB3	2.01	0.43
2:F:207:ASP:OD2	2:F:210:LYS:HB2	2.19	0.43
2:D:168:LYS:HE2	2:D:168:LYS:HB2	1.36	0.43
2:H:61:TYR:HA	2:H:105:GLY:HA3	1.99	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:236:ASN:HD22	2:H:236:ASN:N	2.16	0.43
2:D:7:MET:HB2	2:D:7:MET:HE2	1.83	0.43
2:H:180:GLU:HG2	2:H:235:LYS:HB2	2.00	0.43
1:C:100:LEU:HD23	1:C:100:LEU:HA	1.84	0.43
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.54	0.43
2:F:141:ILE:HG21	2:F:169:LYS:HZ2	1.84	0.43
2:B:84:VAL:O	2:B:85:TYR:HB2	2.18	0.43
2:F:6:PRO:HG3	2:F:195:TRP:CD2	2.54	0.43
2:F:115:LYS:HE3	2:F:117:GLU:HB2	2.00	0.43
2:B:3:GLN:OE1	2:B:195:TRP:CD1	2.72	0.43
2:F:87:SER:HB3	2:F:159:ILE:HD11	2.00	0.43
2:D:14:SER:C	2:D:16:GLU:N	2.70	0.43
2:H:135:GLU:O	2:H:136:ASN:HB2	2.19	0.43
1:C:83:THR:CG2	1:C:86:GLN:HG3	2.23	0.43
1:A:52:ALA:HA	1:A:69:ARG:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ASN:HD21	2:B:234:THR:HG23	1.84	0.43
2:H:152:VAL:CG1	2:H:157:LEU:HD11	2.46	0.43
2:B:166:ILE:HD13	2:B:166:ILE:HG23	1.58	0.43
2:B:171:LEU:HA	2:B:171:LEU:HD12	1.42	0.43
2:B:47:HIS:HB2	2:B:70:ASN:HA	2.01	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
1:E:63:GLY:N	1:E:65:TYR:N	2.66	0.43
2:H:152:VAL:HG13	2:H:152:VAL:O	2.17	0.43
2:B:127:GLN:NE2	2:B:224:LYS:HA	2.34	0.43
2:H:181:THR:HG23	2:H:233:THR:CB	2.48	0.43
1:G:4:VAL:HG12	1:G:109:GLY:HA3	2.00	0.43
1:C:47:HIS:ND1	1:C:57:LYS:HA	2.33	0.43
2:H:7:MET:HE3	2:H:7:MET:HA	2.01	0.43
2:B:134:TYR:CB	3:B:275:HOH:O	2.65	0.43
1:A:87:THR:HG23	1:A:115:SER:C	2.35	0.43
2:H:7:MET:CE	2:H:7:MET:HA	2.48	0.43
2:B:134:TYR:HB3	3:B:275:HOH:O	2.19	0.43
2:H:155:GLN:NE2	2:H:215:TYR:CB	2.76	0.43
2:D:219:LYS:HE2	2:D:221:VAL:CG1	2.49	0.43
1:G:54:SER:HA	2:H:23:ASN:OD1	2.19	0.43
1:A:87:THR:CG2	1:A:115:SER:CA	2.63	0.42
1:G:12:VAL:CG1	1:G:117:LEU:CD1	2.97	0.42
2:F:128:ASN:HA	2:F:145:VAL:O	2.19	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:G:83:THR:O	1:G:116:VAL:HG11	2.20	0.42
1:A:45:LEU:HD23	1:A:58:GLY:HA2	2.00	0.42
2:F:33:VAL:HG23	2:F:88:ASN:HB3	2.02	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:E:93:ALA:HA	1:E:101:TYR:O	2.19	0.42
2:B:101:LYS:C	2:B:103:THR:N	2.73	0.42
2:H:48:ASP:HB2	2:H:66:THR:O	2.19	0.42
2:F:127:GLN:O	2:F:146:GLN:HA	2.19	0.42
1:A:9:ARG:HH22	1:A:111:GLY:N	2.17	0.42
2:F:195:TRP:C	2:F:196:TYR:CD2	2.92	0.42
2:F:165:LEU:O	2:F:166:ILE:C	2.55	0.42
2:H:45:LEU:CD2	2:H:47:HIS:CE1	3.03	0.42
2:D:27:LEU:HD11	2:D:208:GLN:HG2	2.01	0.42
2:F:91:VAL:O	2:F:92:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HE	1:A:44:ARG:HB2	1.47	0.42
2:F:82:VAL:CG1	2:F:113:ILE:CG2	2.93	0.42
2:B:184:ILE:HG13	2:B:230:VAL:CG2	2.48	0.42
1:G:55:THR:O	2:H:23:ASN:ND2	2.49	0.42
2:F:89:TYR:CZ	2:F:209:SER:HB2	2.55	0.42
2:D:2:SER:OG	2:D:192:ASN:OD1	2.23	0.42
2:D:195:TRP:CD2	2:D:195:TRP:O	2.73	0.42
2:B:69:LEU:HD11	2:B:217:ASP:HA	2.02	0.42
2:F:151:SER:HA	2:F:221:VAL:O	2.19	0.42
1:G:17:GLU:O	1:G:82:ALA:N	2.45	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: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
1:C:33:TYR:HB3	1:C:45:LEU:HD11	2.02	0.41
2:H:214:MET:HE3	2:H:215:TYR:CE2	2.56	0.41
2:B:136:ASN:ND2	2:B:234:THR:HG23	2.34	0.41
2:D:94:TYR:CD2	2:D:94:TYR:O	2.74	0.41
2:F:187:ILE:HD11	2:F:229:GLU:CG	2.50	0.41
2:D:181:THR:OG1	2:D:233:THR:OG1	2.38	0.41
2:B:84:VAL:HG12	2:B:85:TYR:N	2.36	0.41
2:F:194:PHE:CE2	2:F:219:LYS:HE3	2.55	0.41
2:B:47:HIS:O	2:B:47:HIS:CD2	2.74	0.41
2:D:65:LYS:HB3	2:D:65:LYS:HE2	1.79	0.41
1:A:67:ALA:O	1:A:68:SER:HB2	2.20	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:C:25:GLN:HG2	1:C:25:GLN:O	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
1:C:32:MET:C	1:C:33:TYR:CD1	2.94	0.41
1:A:62:ASP:HB2	3:A:132:HOH:O	2.19	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:C:31:ASN:HA	1:C:49:SER:O	2.20	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:F:37:LYS:O	2:F:37:LYS:CG	2.65	0.41
2:D:58:LEU:HD22	2:D:58:LEU:HA	1.85	0.41
2:H:91:VAL:O	2:H:92:ASN:HB2	2.20	0.41
2:H:36:THR:O	2:H:37:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:LYS:H	2:F:43:LYS:HD3	1.85	0.41
2:B:27:LEU:C	2:B:31:HIS:HD2	2.24	0.41
2:H:129:VAL:CG1	2:H:130:LEU:N	2.83	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:B:50:ILE:HG21	2:B:50:ILE:HD13	1.85	0.41
1:A:32:MET:HG2	1:A:94:SER:HA	2.03	0.40
1:E:32:MET:HG3	1:E:69:ARG:CZ	2.51	0.40
2:B:135:GLU:O	2:B:136:ASN:HB2	2.21	0.40
2:D:221:VAL:HG21	2:D:226:VAL:HG21	2.03	0.40
2:F:170:ASN:O	2:F:178:PRO:HD3	2.22	0.40
2:H:171:LEU:HD21	2:H:198:MET:HE1	2.00	0.40
2:D:73:LEU:O	2:D:76:LYS:HB3	2.22	0.40
2:H:70:ASN:OD1	2:H:72:ASP:HB2	2.21	0.40
2:H:86:GLY:HA3	2:H:155:GLN:OE1	2.18	0.40
2:F:130:LEU:HD12	2:F:131:VAL:H	1.86	0.40
2:H:166:ILE:HD11	2:H:172:TYR:HD1	1.85	0.40
2:H:103:THR:CG2	2:H:104:GLY:N	2.78	0.40
2:D:3:GLN:HA	2:D:4:PRO:HD3	1.96	0.40
2:H:174:PHE:HD2	2:H:175:ASN:HD22	1.70	0.40
2:H:56:LYS:C	2:H:57:LYS:HD2	2.41	0.40
2:B:186:PHE:O	2:B:193:THR:HA	2.22	0.40
2:F:155:GLN:O	2:F:156:GLU:C	2.59	0.40
2:H:84:VAL:HA	2:H:112:GLY:O	2.21	0.40
2:B:53:ILE:HB	2:B:64:VAL:HG13	2.03	0.40
2:H:82:VAL:HG11	2:H:113:ILE:HG21	2.03	0.40
1:C:69:ARG:NH2	1:C:69:ARG:HG3	2.36	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%)	4	2
1	C	105/112 (94%)	92 (88%)	9 (9%)	4 (4%)	4	2
1	E	107/112 (96%)	83 (78%)	16 (15%)	8 (8%)	1	0
1	G	107/112 (96%)	88 (82%)	16 (15%)	3 (3%)	6	4
2	B	232/237 (98%)	188 (81%)	26 (11%)	18 (8%)	1	0
2	D	231/237 (98%)	175 (76%)	34 (15%)	22 (10%)	1	0
2	F	230/237 (97%)	185 (80%)	31 (14%)	14 (6%)	2	1
2	H	233/237 (98%)	167 (72%)	52 (22%)	14 (6%)	2	1
All	All	1350/1396 (97%)	1069 (79%)	194 (14%)	87 (6%)	2	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

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Mol	Chain	Res	Type
2	B	85	TYR
2	B	102	VAL
2	B	171	LEU
1	C	85	SER
2	D	8	PRO
2	D	75	LYS
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

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Mol	Chain	Res	Type
1	E	85	SER
2	F	137	LYS
2	F	217	ASP
2	H	37	LYS
2	H	218	ASN
2	B	24	MET
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/91 (97%)	78 (89%)	10 (11%)	7 7
1	C	88/91 (97%)	60 (68%)	28 (32%)	0 0
1	E	88/91 (97%)	71 (81%)	17 (19%)	2 1
1	G	88/91 (97%)	67 (76%)	21 (24%)	1 0
2	B	215/217 (99%)	183 (85%)	32 (15%)	4 3
2	D	216/217 (100%)	177 (82%)	39 (18%)	2 2
2	F	215/217 (99%)	159 (74%)	56 (26%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	216/217 (100%)	179 (83%)	37 (17%)	2 2
All	All	1214/1232 (98%)	974 (80%)	240 (20%)	1 1

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	10	ASN
1	A	11	LYS
1	A	36	ARG
1	A	54	SER
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	24	MET
2	B	40	SER
2	B	41	VAL
2	B	56	LYS
2	B	59	LYS
2	B	68	LEU
2	B	75	LYS
2	B	88	ASN
2	B	92	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	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	11	LYS
1	C	18	LYS
1	C	23	CYS
1	C	25	GLN
1	C	26	THR
1	C	27	ASN
1	C	31	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	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	37	LYS
2	D	56	LYS
2	D	57	LYS
2	D	58	LEU
2	D	65	LYS

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Mol	Chain	Res	Type
2	D	68	LEU
2	D	72	ASP
2	D	73	LEU
2	D	78	LYS
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	122	ASP
2	D	125	ASN
2	D	135	GLU
2	D	138	ARG
2	D	139	ASN
2	D	141	ILE
2	D	162	ARG
2	D	168	LYS
2	D	175	ASN
2	D	177	SER
2	D	194	PHE
2	D	204	ASP
2	D	216	ASN
2	D	219	LYS
2	D	220	THR
2	D	224	LYS
1	E	27	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

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Mol	Chain	Res	Type
1	E	74	GLN
1	E	85	SER
1	E	88	SER
1	E	99	THR
1	E	115	SER
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
2	F	103	THR
2	F	109	MET
2	F	115	LYS
2	F	116	HIS
2	F	117	GLU
2	F	123	ASN
2	F	129	VAL
2	F	138	ARG
2	F	139	ASN
2	F	140	THR

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Mol	Chain	Res	Type
2	F	141	ILE
2	F	145	VAL
2	F	150	LYS
2	F	151	SER
2	F	157	LEU
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	194	PHE
2	F	198	MET
2	F	205	LYS
2	F	216	ASN
2	F	218	ASN
2	F	224	LYS
2	F	233	THR
2	F	234	THR
2	F	236	ASN
1	G	6	GLN
1	G	9	ARG
1	G	14	VAL
1	G	17	GLU
1	G	18	LYS
1	G	21	LEU
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	86	GLN
1	G	89	VAL
1	G	92	CYS
1	G	99	THR
2	H	2	SER

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Mol	Chain	Res	Type
2	H	7	MET
2	H	9	ASP
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	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
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	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	229	GLU
2	H	236	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	ASN

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Mol	Chain	Res	Type
1	A	31	ASN
1	A	74	GLN
2	B	31	HIS
2	B	88	ASN
2	B	139	ASN
2	B	155	GLN
2	B	175	ASN
2	B	189	ASN
2	B	190	ASN
2	B	216	ASN
1	C	10	ASN
1	C	24	GLN
1	C	30	ASN
1	C	37	GLN
1	C	72	GLN
1	C	74	GLN
2	D	3	GLN
2	D	47	HIS
2	D	88	ASN
2	D	92	ASN
2	D	127	GLN
2	D	128	ASN
2	D	136	ASN
2	D	163	ASN
2	D	167	ASN
2	D	170	ASN
2	D	216	ASN
1	E	24	GLN
2	F	3	GLN
2	F	92	ASN
2	F	216	ASN
2	F	236	ASN
1	G	31	ASN
1	G	41	HIS
2	H	31	HIS
2	H	88	ASN
2	H	120	HIS
2	H	146	GLN
2	H	170	ASN
2	H	175	ASN
2	H	189	ASN
2	H	192	ASN

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Mol	Chain	Res	Type
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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.24	1 (0%) 85 89	8, 35, 52, 59	0
1	C	109/112 (97%)	-0.22	1 (0%) 85 89	21, 39, 58, 66	0
1	E	109/112 (97%)	-0.13	1 (0%) 85 89	27, 47, 64, 70	0
1	G	109/112 (97%)	-0.15	0 100 100	24, 40, 59, 63	0
2	B	234/237 (98%)	-0.26	1 (0%) 93 95	10, 41, 65, 86	0
2	D	235/237 (99%)	-0.13	4 (1%) 73 79	23, 47, 71, 87	0
2	F	234/237 (98%)	-0.22	1 (0%) 93 95	29, 45, 75, 91	0
2	H	237/237 (100%)	-0.01	5 (2%) 67 74	27, 50, 76, 103	0
All	All	1376/1396 (98%)	-0.16	14 (1%) 84 88	8, 44, 69, 103	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	237	GLY	5.3
2	H	102	VAL	4.2
2	H	1	GLU	3.7
2	D	237	GLY	3.7
2	H	103	THR	3.6
1	A	2	ALA	3.4
1	C	2	ALA	3.3
1	E	2	ALA	3.1
2	D	97	SER	3.0
2	H	235	LYS	2.7
2	B	99	ASP	2.6
2	F	96	SER	2.6
2	D	2	SER	2.2
2	D	3	GLN	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.