



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:20 AM UTC

PDB ID : 4QF6 / pdb_00004qf6
Title : Structure of Aldehyde Dehydrogenase from Bacillus cereus, E194S mutant
Authors : Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2014-05-19
Resolution : 1.90 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:

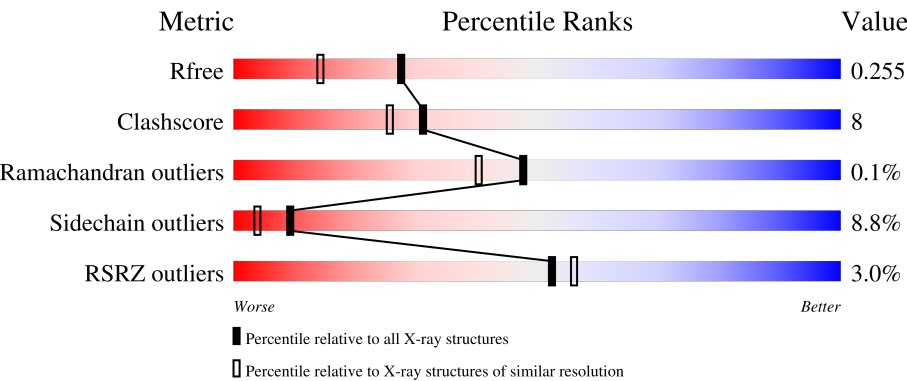
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	494	% 79% 17% ...
1	B	494	2% 81% 14% ..
1	C	494	% 82% 14% ..
1	D	494	% 80% 16% ..
1	E	494	2% 83% 14% ...

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Mol	Chain	Length	Quality of chain
1	F	494	2% 76% 20%
1	G	494	3% 79% 17%
1	H	494	2% 77% 16% 5%
1	I	494	2% 78% 18%
1	J	494	4% 77% 16% 6%
1	K	494	6% 72% 22% 5%
1	L	494	9% 68% 24% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47191 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	B	491	Total	C	N	O	S	0	1	0
			3791	2414	630	733	14			
1	C	491	Total	C	N	O	S	0	1	0
			3793	2415	630	734	14			
1	D	489	Total	C	N	O	S	0	3	0
			3787	2413	628	732	14			
1	E	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	F	491	Total	C	N	O	S	0	2	0
			3794	2416	630	734	14			
1	G	490	Total	C	N	O	S	0	0	0
			3781	2408	629	730	14			
1	H	490	Total	C	N	O	S	0	1	0
			3787	2412	629	732	14			
1	I	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	J	491	Total	C	N	O	S	0	0	0
			3788	2412	630	732	14			
1	K	489	Total	C	N	O	S	0	0	0
			3773	2404	627	728	14			
1	L	488	Total	C	N	O	S	0	0	0
			3764	2398	626	726	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	SER	GLU	engineered mutation	UNP C2N217
B	194	SER	GLU	engineered mutation	UNP C2N217
C	194	SER	GLU	engineered mutation	UNP C2N217
D	194	SER	GLU	engineered mutation	UNP C2N217
E	194	SER	GLU	engineered mutation	UNP C2N217

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Chain	Residue	Modelled	Actual	Comment	Reference
F	194	SER	GLU	engineered mutation	UNP C2N217
G	194	SER	GLU	engineered mutation	UNP C2N217
H	194	SER	GLU	engineered mutation	UNP C2N217
I	194	SER	GLU	engineered mutation	UNP C2N217
J	194	SER	GLU	engineered mutation	UNP C2N217
K	194	SER	GLU	engineered mutation	UNP C2N217
L	194	SER	GLU	engineered mutation	UNP C2N217

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	D	2	Total Na 2 2	0	0
2	E	2	Total Na 2 2	0	0
2	F	2	Total Na 2 2	0	0
2	G	2	Total Na 2 2	0	0
2	H	2	Total Na 2 2	0	0
2	I	2	Total Na 2 2	0	0
2	J	2	Total Na 2 2	0	0
2	K	2	Total Na 2 2	0	0
2	L	2	Total Na 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	255	Total O 255 255	0	0
3	B	123	Total O 123 123	0	0

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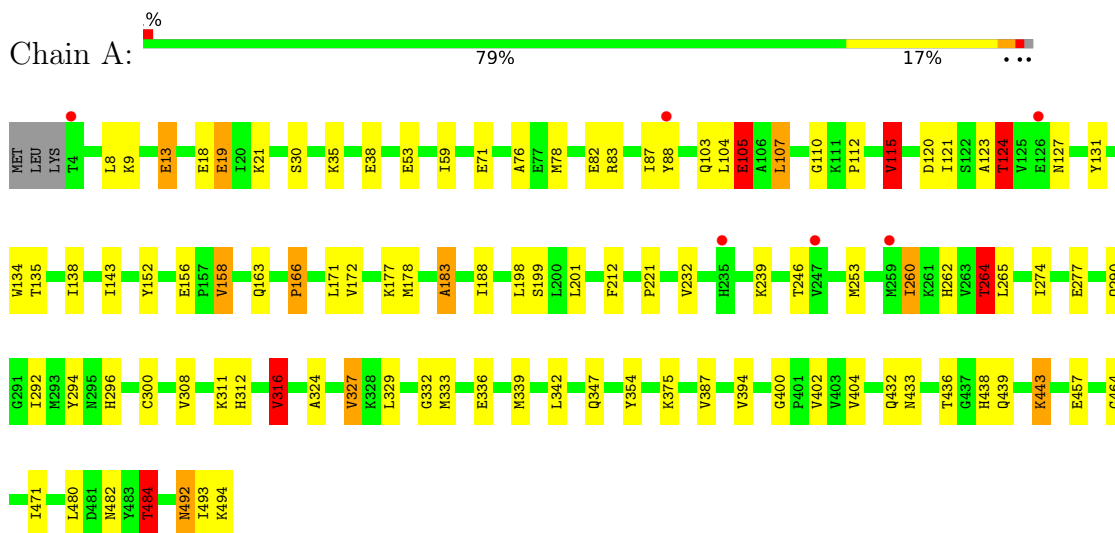
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	197	Total 197	O 197	0	0
3	D	216	Total 216	O 216	0	0
3	E	218	Total 218	O 218	0	0
3	F	124	Total 124	O 124	0	0
3	G	152	Total 152	O 152	0	0
3	H	143	Total 143	O 143	0	0
3	I	109	Total 109	O 109	0	0
3	J	74	Total 74	O 74	0	0
3	K	76	Total 76	O 76	0	0
3	L	62	Total 62	O 62	0	0

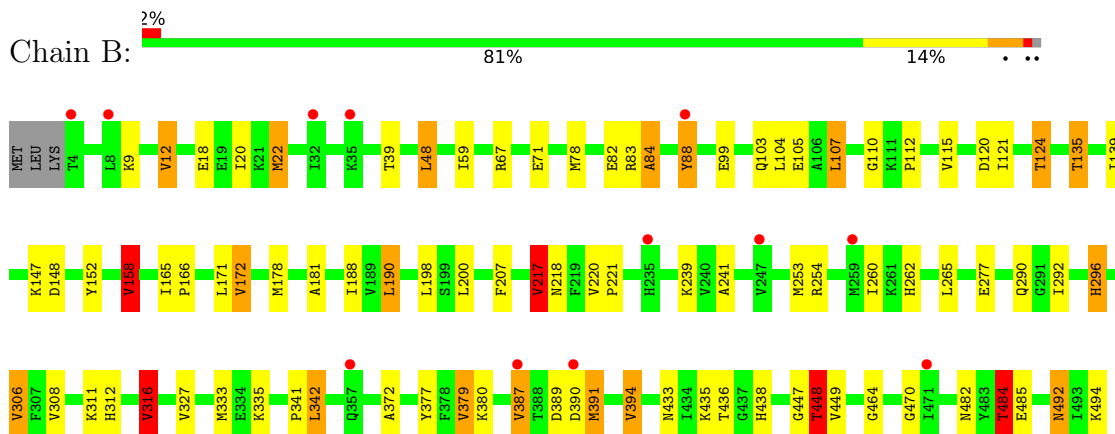
3 Residue-property plots [i](#)

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.

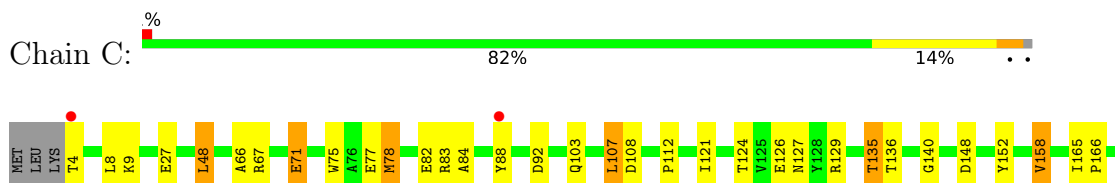
- Molecule 1: Aldehyde dehydrogenase

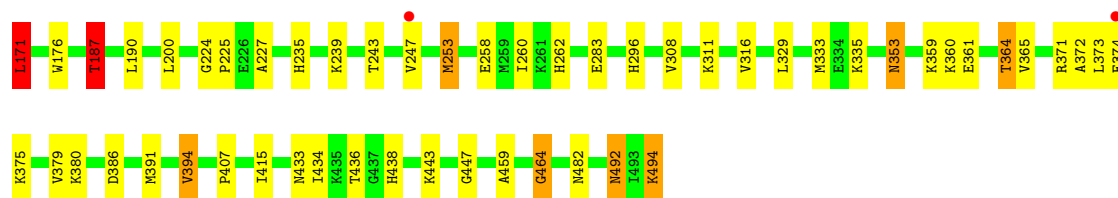


- Molecule 1: Aldehyde dehydrogenase

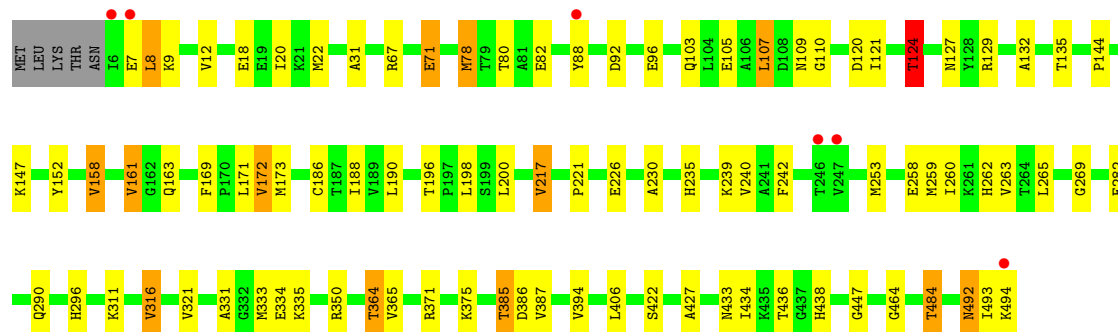
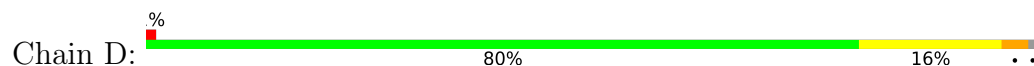


- Molecule 1: Aldehyde dehydrogenase

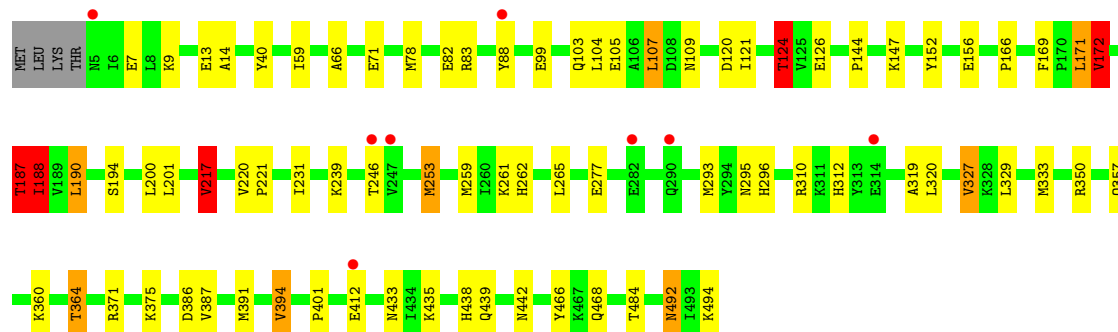
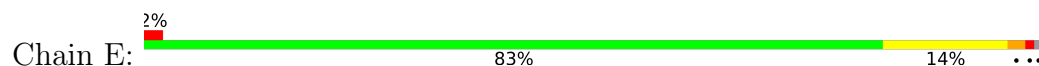




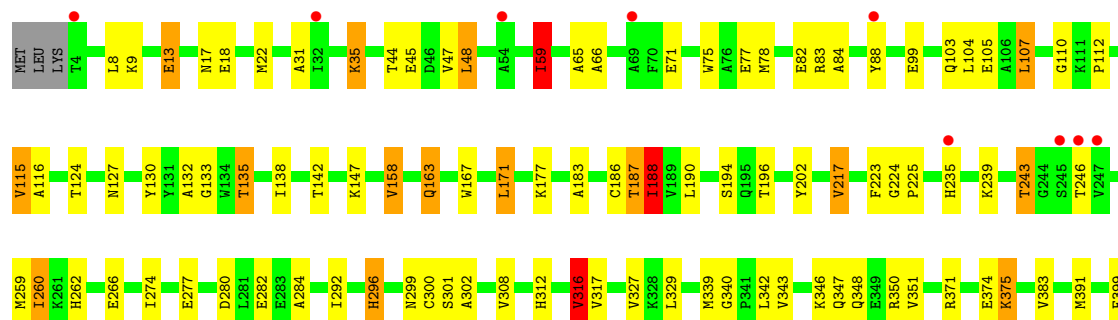
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase

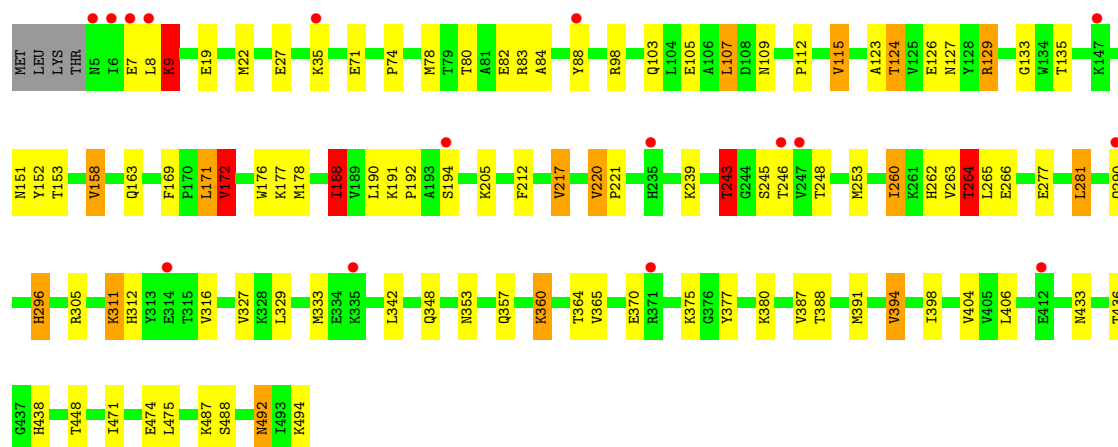
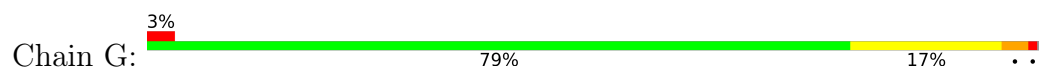


• Molecule 1: Aldehyde dehydrogenase

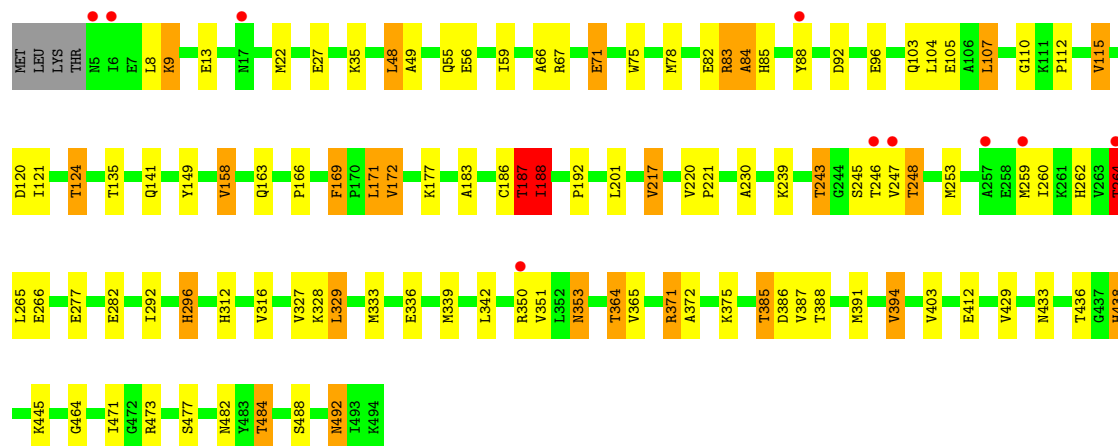
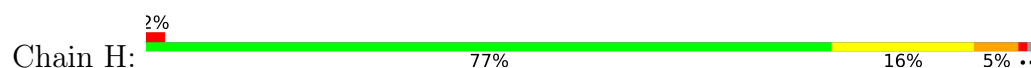




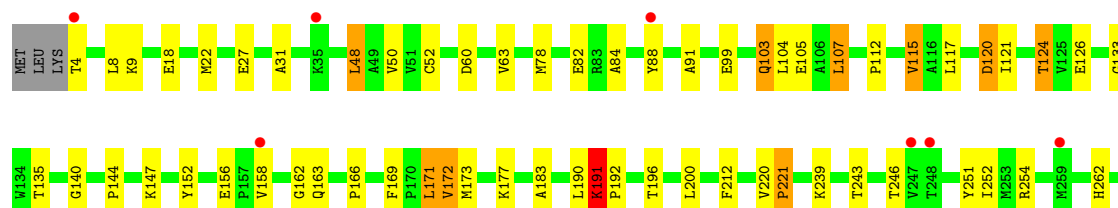
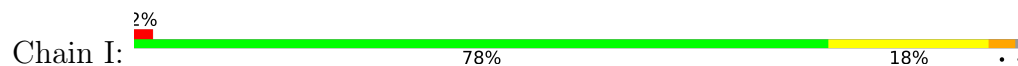
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase

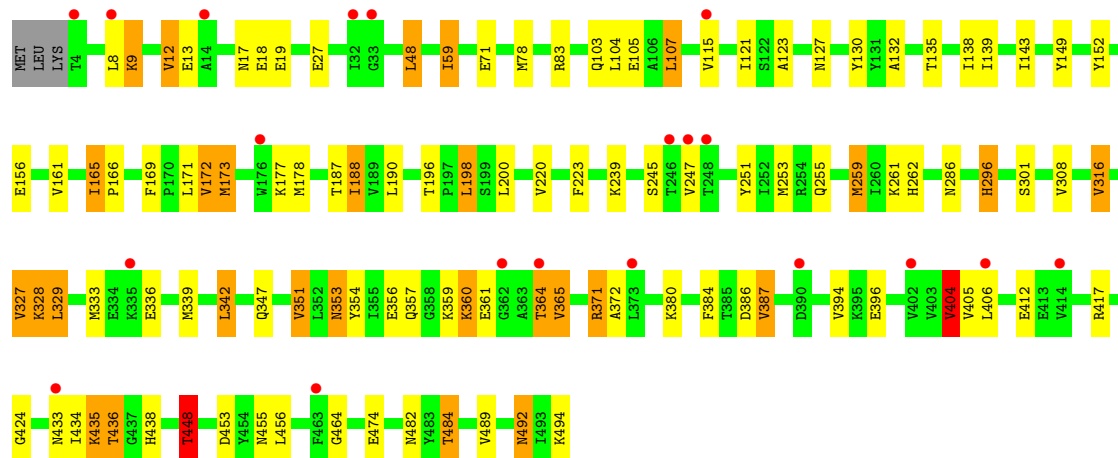
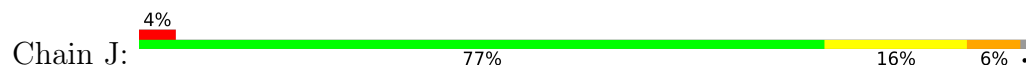


• Molecule 1: Aldehyde dehydrogenase





• Molecule 1: Aldehyde dehydrogenase

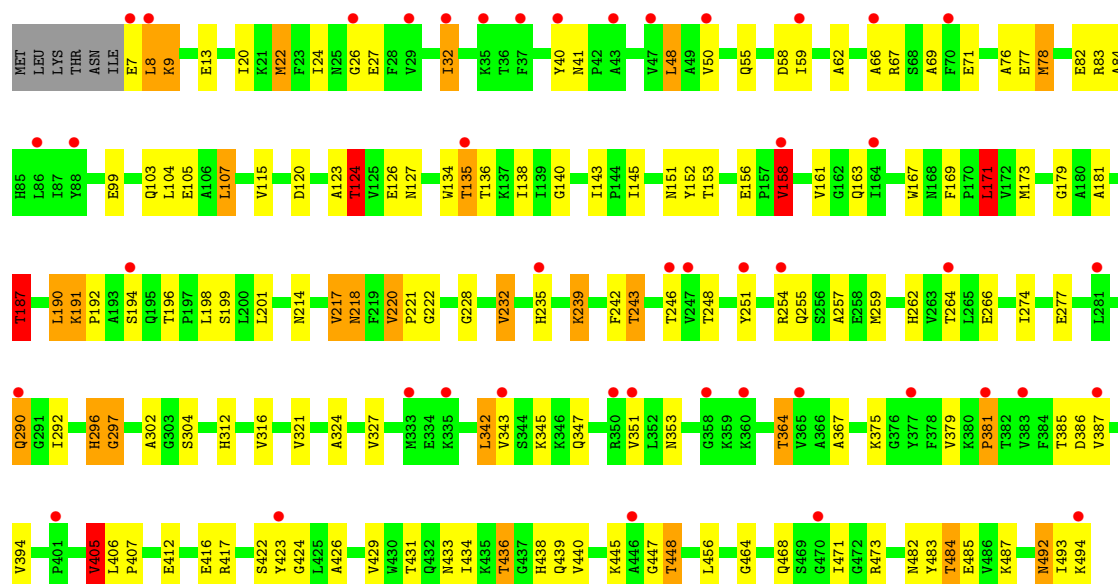


• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.56Å 93.66Å 247.85Å 90.00° 95.55° 90.00°	Depositor
Resolution (Å)	43.56 – 1.90 43.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.9 (43.56-1.90) 84.9 (43.56-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.47 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.252 0.211 , 0.255	Depositor DCC
R_{free} test set	22144 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtrriage
Anisotropy	0.226	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	47191	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3627e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.48	23/3873 (0.6%)	1.31	18/5254 (0.3%)
1	B	1.36	13/3873 (0.3%)	1.30	19/5254 (0.4%)
1	C	1.40	10/3875 (0.3%)	1.26	13/5257 (0.2%)
1	D	1.42	15/3875 (0.4%)	1.30	26/5256 (0.5%)
1	E	1.46	11/3860 (0.3%)	1.26	21/5236 (0.4%)
1	F	1.41	19/3879 (0.5%)	1.31	21/5262 (0.4%)
1	G	1.39	15/3860 (0.4%)	1.25	13/5236 (0.2%)
1	H	1.32	6/3869 (0.2%)	1.30	23/5248 (0.4%)
1	I	1.30	11/3867 (0.3%)	1.23	11/5246 (0.2%)
1	J	1.27	9/3867 (0.2%)	1.27	22/5246 (0.4%)
1	K	1.37	22/3852 (0.6%)	1.26	8/5225 (0.2%)
1	L	1.38	22/3843 (0.6%)	1.32	20/5214 (0.4%)
All	All	1.38	176/46393 (0.4%)	1.28	215/62934 (0.3%)

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	D	0	1

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	163	GLN	C-O	-8.59	1.13	1.23
1	G	264	THR	CB-CG2	8.18	1.79	1.52
1	E	401	PRO	CA-C	-7.96	1.46	1.53
1	K	271	SER	CA-C	-7.94	1.44	1.53
1	I	169	PHE	N-CA	7.71	1.54	1.46
1	B	484	THR	N-CA	-7.59	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	165	ILE	C-O	7.51	1.30	1.24
1	L	196	THR	N-CA	7.36	1.54	1.46
1	G	260	ILE	N-CA	7.25	1.55	1.46
1	F	383	VAL	C-O	7.20	1.32	1.24
1	I	133	GLY	N-CA	7.08	1.55	1.45
1	H	264	THR	CB-CG2	7.03	1.75	1.52
1	L	220	VAL	N-CA	6.96	1.55	1.46
1	K	195	GLN	C-O	6.81	1.32	1.24
1	B	112	PRO	C-O	6.79	1.31	1.23
1	C	176	TRP	N-CA	6.77	1.54	1.46
1	K	208	LYS	C-O	-6.75	1.16	1.24
1	L	274	ILE	C-O	6.74	1.31	1.24
1	A	484	THR	CB-CG2	-6.70	1.30	1.52
1	K	131	TYR	CA-CB	6.69	1.64	1.53
1	E	484	THR	CB-CG2	-6.63	1.30	1.52
1	J	489	VAL	C-O	6.58	1.31	1.24
1	K	439	GLN	C-O	-6.54	1.16	1.24
1	K	188	ILE	CA-C	6.52	1.60	1.52
1	I	52	CYS	CA-C	6.45	1.61	1.52
1	E	126	GLU	C-O	-6.45	1.16	1.24
1	H	484	THR	N-CA	-6.45	1.38	1.46
1	C	187	THR	CB-CG2	-6.35	1.31	1.52
1	B	22	MET	CA-C	-6.35	1.44	1.53
1	E	320	LEU	C-O	-6.32	1.16	1.24
1	J	464	GLY	N-CA	6.31	1.51	1.45
1	F	342	LEU	N-CA	-6.30	1.37	1.45
1	A	19	GLU	C-O	-6.29	1.16	1.23
1	K	418	ALA	C-O	6.27	1.31	1.24
1	B	448	THR	CB-CG2	-6.26	1.31	1.52
1	D	230	ALA	CA-C	6.24	1.60	1.52
1	B	181	ALA	N-CA	-6.22	1.39	1.46
1	D	406	LEU	CA-C	-6.22	1.47	1.52
1	L	218	ASN	N-CA	6.18	1.53	1.46
1	F	116	ALA	C-O	-6.18	1.17	1.24
1	G	151	ASN	C-O	-6.13	1.17	1.24
1	C	283	GLU	C-O	-6.11	1.16	1.24
1	A	260	ILE	C-O	6.07	1.31	1.24
1	I	103	GLN	C-O	-6.06	1.17	1.24
1	L	302	ALA	N-CA	6.05	1.53	1.46
1	D	129	ARG	N-CA	6.03	1.53	1.46
1	L	181	ALA	C-O	5.99	1.30	1.24
1	F	158	VAL	N-CA	5.96	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	260	ILE	C-O	5.95	1.31	1.24
1	F	347	GLN	C-O	-5.95	1.17	1.24
1	F	348	GLN	CA-C	5.91	1.60	1.52
1	L	124	THR	CA-CB	5.91	1.62	1.53
1	C	243	THR	CA-C	5.90	1.59	1.52
1	D	484	THR	CB-CG2	-5.89	1.33	1.52
1	A	166	PRO	N-CA	-5.88	1.40	1.47
1	K	162	GLY	CA-C	-5.88	1.48	1.52
1	A	457	GLU	C-O	5.88	1.31	1.23
1	A	339	MET	C-O	5.87	1.30	1.23
1	A	183	ALA	N-CA	5.85	1.53	1.46
1	J	143	ILE	N-CA	-5.84	1.41	1.46
1	A	294	TYR	C-O	5.84	1.30	1.23
1	J	448	THR	CB-CG2	-5.84	1.33	1.52
1	D	263	VAL	C-O	5.83	1.30	1.24
1	K	100	GLU	N-CA	-5.83	1.39	1.46
1	C	108	ASP	C-O	5.83	1.30	1.24
1	B	110	GLY	N-CA	5.81	1.51	1.45
1	B	84	ALA	C-O	5.80	1.30	1.24
1	A	404	VAL	C-O	-5.79	1.16	1.24
1	D	12	VAL	N-CA	5.75	1.53	1.46
1	A	143	ILE	CA-C	5.75	1.58	1.52
1	K	273	ASN	C-O	5.72	1.30	1.24
1	D	186	CYS	N-CA	5.71	1.53	1.45
1	F	186	CYS	N-CA	5.70	1.53	1.45
1	E	14	ALA	C-O	-5.68	1.17	1.24
1	J	130	TYR	C-O	5.65	1.30	1.24
1	A	332	GLY	N-CA	5.65	1.53	1.45
1	F	65	ALA	C-O	-5.64	1.17	1.24
1	D	8	LEU	N-CA	5.63	1.52	1.46
1	K	174	SER	C-O	5.63	1.30	1.24
1	H	192	PRO	CA-C	-5.62	1.46	1.52
1	A	400	GLY	C-O	5.62	1.31	1.24
1	G	365	VAL	CA-C	-5.61	1.46	1.53
1	J	456	LEU	C-O	-5.61	1.17	1.24
1	H	22	MET	C-O	5.60	1.30	1.23
1	I	144	PRO	C-O	-5.60	1.19	1.24
1	I	251	TYR	N-CA	5.59	1.53	1.46
1	K	108	ASP	C-O	5.59	1.30	1.24
1	F	292	ILE	CA-C	5.58	1.58	1.52
1	F	466	TYR	C-O	-5.58	1.16	1.23
1	L	423	TYR	N-CA	5.56	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	133	GLY	N-CA	5.55	1.53	1.45
1	I	196	THR	C-O	5.55	1.30	1.23
1	C	148	ASP	C-O	-5.55	1.16	1.24
1	B	241	ALA	C-O	-5.54	1.17	1.23
1	F	292	ILE	C-O	5.54	1.29	1.23
1	A	300	CYS	C-O	-5.54	1.17	1.24
1	C	140	GLY	C-O	5.54	1.29	1.24
1	D	226	GLU	CA-C	5.52	1.56	1.52
1	E	166	PRO	N-CA	-5.51	1.40	1.47
1	L	217	VAL	CA-C	5.51	1.59	1.52
1	K	187	THR	CB-CG2	-5.51	1.34	1.52
1	A	274	ILE	C-O	5.48	1.30	1.24
1	H	166	PRO	N-CA	-5.48	1.40	1.47
1	I	140	GLY	N-CA	5.47	1.50	1.44
1	D	240	VAL	CA-CB	5.45	1.61	1.54
1	L	143	ILE	CA-C	-5.44	1.47	1.52
1	J	484	THR	CA-C	5.44	1.59	1.52
1	G	260	ILE	C-O	5.43	1.30	1.24
1	I	162	GLY	C-O	5.43	1.29	1.23
1	J	453	ASP	C-O	-5.43	1.19	1.24
1	D	242	PHE	C-O	5.42	1.30	1.23
1	L	304	SER	N-CA	5.41	1.53	1.46
1	C	464	GLY	N-CA	5.41	1.50	1.45
1	K	126	GLU	C-O	-5.41	1.17	1.24
1	G	243	THR	CB-CG2	-5.40	1.34	1.52
1	L	69	ALA	N-CA	5.40	1.53	1.46
1	D	198	LEU	N-CA	-5.38	1.39	1.46
1	K	40	TYR	CA-C	-5.38	1.46	1.52
1	I	221	PRO	CA-C	5.38	1.59	1.52
1	K	125	VAL	N-CA	5.34	1.52	1.46
1	F	183	ALA	N-CA	5.33	1.52	1.46
1	G	129	ARG	N-CA	5.32	1.52	1.46
1	B	292	ILE	N-CA	5.32	1.53	1.46
1	G	398	ILE	C-O	5.29	1.30	1.23
1	L	439	GLN	N-CA	5.29	1.52	1.46
1	B	449	VAL	C-O	-5.29	1.18	1.24
1	E	187	THR	CB-CG2	-5.28	1.35	1.52
1	J	417	ARG	C-O	-5.27	1.17	1.24
1	G	305	ARG	C-O	-5.27	1.17	1.24
1	A	347	GLN	C-O	-5.27	1.17	1.24
1	G	281	LEU	N-CA	-5.26	1.40	1.46
1	L	169	PHE	N-CA	5.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	145	ILE	N-CA	5.25	1.50	1.46
1	G	172	VAL	CA-CB	5.24	1.61	1.54
1	K	461	ALA	C-O	5.24	1.30	1.24
1	D	144	PRO	C-O	-5.23	1.19	1.24
1	I	196	THR	N-CA	5.23	1.52	1.46
1	C	92	ASP	CA-C	5.23	1.59	1.52
1	G	220	VAL	N-CA	5.22	1.52	1.46
1	G	488	SER	C-O	5.22	1.30	1.24
1	K	117	LEU	N-CA	5.21	1.52	1.46
1	F	130	TYR	C-O	5.19	1.30	1.24
1	G	80	THR	C-O	-5.18	1.18	1.24
1	F	13	GLU	N-CA	5.18	1.52	1.46
1	A	19	GLU	CD-OE1	5.18	1.35	1.25
1	B	218	ASN	N-CA	5.17	1.52	1.46
1	E	295	ASN	CA-C	-5.17	1.45	1.53
1	A	105	GLU	CA-C	5.17	1.59	1.52
1	L	62	ALA	C-O	5.17	1.30	1.24
1	L	40	TYR	C-O	5.16	1.30	1.23
1	D	172	VAL	N-CA	5.15	1.52	1.46
1	A	246	THR	CA-C	-5.12	1.46	1.52
1	C	329	LEU	N-CA	-5.12	1.39	1.46
1	F	442	ASN	CG-OD1	5.11	1.33	1.23
1	G	133	GLY	C-O	5.11	1.30	1.23
1	A	53	GLU	C-O	-5.10	1.18	1.24
1	L	456	LEU	N-CA	5.09	1.52	1.46
1	A	402	VAL	C-O	-5.09	1.18	1.24
1	L	77	GLU	CA-C	5.09	1.59	1.52
1	A	480	LEU	CA-C	-5.08	1.45	1.52
1	K	226	GLU	CA-C	5.07	1.56	1.52
1	B	67	ARG	C-O	-5.06	1.18	1.24
1	L	242	PHE	C-O	5.06	1.30	1.23
1	L	416	GLU	C-O	-5.06	1.18	1.24
1	E	144	PRO	N-CA	-5.05	1.42	1.47
1	L	171	LEU	CA-C	5.05	1.59	1.52
1	E	217	VAL	C-O	5.05	1.29	1.24
1	E	40	TYR	C-O	5.04	1.30	1.23
1	B	39	THR	CA-CB	5.04	1.62	1.53
1	D	269	GLY	N-CA	-5.03	1.40	1.45
1	H	186	CYS	N-CA	5.03	1.52	1.45
1	L	179	GLY	N-CA	5.03	1.52	1.45
1	A	232	VAL	N-CA	5.02	1.52	1.46
1	F	391	MET	C-O	5.01	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	GLY	CA-C	-5.01	1.46	1.51
1	K	158	VAL	N-CA	5.00	1.52	1.46

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	VAL	CB-CA-C	-11.19	93.92	112.16
1	A	158	VAL	CB-CA-C	-10.41	96.02	112.16
1	L	158	VAL	CB-CA-C	-8.74	100.79	111.97
1	H	158	VAL	CB-CA-C	-8.19	101.08	112.14
1	E	187	THR	OG1-CB-CG2	8.13	125.56	109.30
1	G	188	ILE	N-CA-C	7.90	120.14	108.45
1	H	187	THR	N-CA-CB	-7.87	97.86	111.55
1	D	217	VAL	N-CA-CB	-7.83	100.08	111.52
1	C	158	VAL	CB-CA-C	-7.71	101.72	112.14
1	D	217	VAL	CB-CA-C	7.50	121.28	110.33
1	K	158	VAL	CB-CA-C	-7.45	101.93	112.22
1	D	335	LYS	N-CA-C	7.38	120.20	111.71
1	K	188	ILE	N-CA-C	7.35	119.41	108.46
1	H	188	ILE	N-CA-C	7.29	119.25	108.45
1	B	389	ASP	CA-C-N	7.14	129.85	120.28
1	B	389	ASP	C-N-CA	7.14	129.85	120.28
1	A	316	VAL	N-CA-CB	7.08	121.20	110.58
1	A	124	THR	OG1-CB-CG2	7.04	123.38	109.30
1	F	316	VAL	N-CA-C	7.04	117.83	110.72
1	A	292	ILE	N-CA-C	6.86	117.83	111.45
1	D	80	THR	N-CA-C	6.85	119.59	111.71
1	L	405	VAL	CB-CA-C	6.84	120.48	110.77
1	E	293	MET	N-CA-C	6.83	119.75	111.82
1	D	385	THR	N-CA-CB	-6.78	99.99	111.31
1	L	158	VAL	N-CA-CB	6.77	118.47	110.55
1	I	91	ALA	N-CA-C	-6.75	104.00	111.36
1	C	353	ASN	N-CA-C	6.72	118.61	111.28
1	L	135	THR	CB-CA-C	-6.70	99.29	110.68
1	B	158	VAL	CB-CA-C	-6.67	102.32	112.05
1	L	20	ILE	CB-CA-C	-6.66	102.79	111.25
1	G	158	VAL	CB-CA-C	-6.63	101.51	112.26
1	H	169	PHE	CA-C-N	-6.61	111.57	119.84
1	H	169	PHE	C-N-CA	-6.61	111.57	119.84
1	A	110	GLY	N-CA-C	6.56	120.59	113.58
1	E	121	ILE	CB-CA-C	-6.53	103.21	112.22
1	H	110	GLY	N-CA-C	6.39	123.23	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	THR	OG1-CB-CG2	6.37	122.04	109.30
1	B	306	VAL	N-CA-CB	6.36	119.36	111.41
1	D	124	THR	CB-CA-C	6.35	120.93	110.90
1	H	220	VAL	CA-C-N	6.33	126.85	120.14
1	H	220	VAL	C-N-CA	6.33	126.85	120.14
1	E	466	TYR	N-CA-C	-6.32	102.38	110.53
1	C	187	THR	N-CA-CB	-6.31	100.56	111.55
1	J	132	ALA	N-CA-C	-6.31	104.40	111.28
1	J	404	VAL	N-CA-CB	-6.31	102.70	111.41
1	L	120	ASP	N-CA-C	6.30	118.67	111.11
1	L	440	VAL	N-CA-C	-6.29	104.36	110.72
1	G	353	ASN	N-CA-C	6.26	118.10	111.28
1	E	217	VAL	CA-CB-CG1	6.26	121.04	110.40
1	D	196	THR	N-CA-C	6.24	118.60	109.30
1	G	217	VAL	N-CA-CB	-6.23	101.22	111.44
1	D	78	MET	CG-SD-CE	-6.22	87.21	100.90
1	E	187	THR	N-CA-CB	-6.17	100.81	111.55
1	L	55	GLN	N-CA-C	-6.16	101.08	109.95
1	B	198	LEU	N-CA-C	6.14	117.64	111.07
1	J	353	ASN	N-CA-C	6.13	117.97	111.28
1	I	172	VAL	CB-CA-C	-6.13	104.01	112.04
1	F	110	GLY	N-CA-C	6.08	122.03	114.37
1	J	156	GLU	CA-C-N	-6.07	113.51	119.76
1	J	156	GLU	C-N-CA	-6.07	113.51	119.76
1	E	156	GLU	CA-C-N	-6.06	113.53	119.78
1	E	156	GLU	C-N-CA	-6.06	113.53	119.78
1	E	172	VAL	N-CA-CB	6.04	118.75	110.54
1	A	354	TYR	N-CA-C	6.02	117.51	111.07
1	K	165	ILE	N-CA-C	6.00	115.80	109.01
1	H	217	VAL	N-CA-CB	-6.00	102.77	111.52
1	J	286	ASN	N-CA-C	5.99	117.48	111.07
1	L	217	VAL	N-CA-CB	-5.99	102.78	111.52
1	F	217	VAL	N-CA-CB	-5.99	101.88	111.58
1	I	191	LYS	CA-C-N	-5.98	114.47	120.21
1	I	191	LYS	C-N-CA	-5.98	114.47	120.21
1	A	212	PHE	CA-C-N	-5.97	113.53	119.92
1	A	212	PHE	C-N-CA	-5.97	113.53	119.92
1	E	188	ILE	N-CA-C	5.96	117.27	108.45
1	E	217	VAL	N-CA-CB	-5.95	101.67	111.44
1	L	217	VAL	CB-CA-C	5.95	119.02	110.33
1	H	9	LYS	CA-C-N	5.95	127.27	119.84
1	H	9	LYS	C-N-CA	5.95	127.27	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	217	VAL	CA-CB-CG1	5.90	120.43	110.40
1	E	124	THR	OG1-CB-CG2	5.88	121.06	109.30
1	L	297	GLY	N-CA-C	-5.85	107.81	115.47
1	G	212	PHE	CA-C-N	-5.85	114.24	120.03
1	G	212	PHE	C-N-CA	-5.85	114.24	120.03
1	I	63	VAL	N-CA-CB	5.84	116.99	110.51
1	K	231	ILE	N-CA-C	-5.83	105.05	110.53
1	B	217	VAL	CB-CA-C	5.83	120.79	110.71
1	J	327	VAL	N-CA-CB	5.82	117.47	110.31
1	I	212	PHE	CA-C-N	-5.82	113.79	119.78
1	I	212	PHE	C-N-CA	-5.82	113.79	119.78
1	B	165	ILE	N-CA-C	5.81	115.42	108.45
1	C	78	MET	N-CA-CB	-5.80	101.81	110.17
1	H	471	ILE	N-CA-C	-5.80	99.14	107.78
1	I	465	GLY	N-CA-C	5.79	121.61	111.25
1	B	172	VAL	CB-CA-C	-5.78	104.48	111.88
1	B	217	VAL	N-CA-CB	-5.77	101.98	111.45
1	H	353	ASN	N-CA-C	5.76	117.56	111.28
1	J	455	ASN	N-CA-C	5.72	119.56	112.24
1	F	47	VAL	N-CA-C	-5.70	101.67	109.37
1	H	264	THR	CB-CA-C	5.70	120.94	109.38
1	F	13	GLU	CB-CA-C	-5.66	102.00	110.88
1	D	316	VAL	N-CA-CB	5.65	119.06	110.58
1	F	158	VAL	CB-CA-C	-5.65	103.40	112.16
1	J	484	THR	OG1-CB-CG2	5.65	120.59	109.30
1	D	135	THR	CB-CA-C	-5.64	101.09	110.68
1	D	158	VAL	N-CA-CB	5.64	121.61	110.95
1	D	124	THR	CA-CB-OG1	5.64	118.05	109.60
1	A	156	GLU	CA-C-N	-5.63	114.13	119.76
1	A	156	GLU	C-N-CA	-5.63	114.13	119.76
1	J	135	THR	CB-CA-C	-5.63	100.22	110.63
1	F	300	CYS	CA-CB-SG	-5.62	101.47	114.40
1	J	223	PHE	CA-C-N	5.62	125.23	121.13
1	J	223	PHE	C-N-CA	5.62	125.23	121.13
1	G	264	THR	CB-CA-C	5.61	120.09	109.37
1	A	124	THR	CA-CB-OG1	5.60	118.00	109.60
1	E	327	VAL	CA-CB-CG1	5.60	119.92	110.40
1	C	187	THR	N-CA-C	-5.59	100.85	109.52
1	D	132	ALA	CA-C-N	5.56	126.26	120.03
1	D	132	ALA	C-N-CA	5.56	126.26	120.03
1	B	391	MET	N-CA-C	5.56	118.29	110.23
1	I	117	LEU	N-CA-C	5.56	117.02	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	120	ASP	N-CA-C	5.56	117.02	111.07
1	D	427	ALA	CA-C-N	5.52	125.41	121.65
1	D	427	ALA	C-N-CA	5.52	125.41	121.65
1	C	227	ALA	N-CA-C	5.50	116.95	111.07
1	F	405	VAL	CB-CA-C	5.48	118.56	110.77
1	G	9	LYS	CA-C-N	5.48	126.69	119.84
1	G	9	LYS	C-N-CA	5.48	126.69	119.84
1	D	385	THR	OG1-CB-CG2	5.46	120.23	109.30
1	A	198	LEU	N-CA-C	5.45	117.02	111.14
1	H	385	THR	N-CA-CB	-5.44	102.81	111.62
1	B	484	THR	CB-CA-C	5.43	120.11	109.35
1	J	342	LEU	N-CA-C	-5.43	103.52	110.53
1	K	460	ALA	N-CA-C	5.42	119.88	113.16
1	A	316	VAL	CG1-CB-CG2	5.42	122.72	110.80
1	A	131	TYR	N-CA-C	5.42	118.10	111.82
1	A	264	THR	CB-CA-C	5.41	119.62	109.71
1	E	187	THR	CA-CB-OG1	5.41	117.71	109.60
1	B	448	THR	OG1-CB-CG2	5.40	120.11	109.30
1	E	442	ASN	N-CA-C	5.39	117.16	111.28
1	F	224	GLY	CA-C-N	5.39	125.22	119.28
1	F	224	GLY	C-N-CA	5.39	125.22	119.28
1	B	470	GLY	N-CA-C	5.38	118.61	110.75
1	B	88	TYR	CA-CB-CG	-5.38	104.22	113.90
1	H	187	THR	OG1-CB-CG2	5.38	120.05	109.30
1	J	165	ILE	N-CA-C	5.37	113.80	107.84
1	F	135	THR	CB-CA-C	-5.37	101.88	110.79
1	L	347	GLN	N-CA-C	5.37	117.21	111.36
1	B	316	VAL	N-CA-CB	5.36	121.09	110.95
1	D	31	ALA	N-CA-C	-5.36	102.95	110.50
1	B	39	THR	N-CA-C	-5.35	101.45	109.95
1	E	319	ALA	N-CA-C	5.34	116.78	111.07
1	J	196	THR	CA-C-N	5.34	125.03	119.64
1	J	196	THR	C-N-CA	5.34	125.03	119.64
1	J	484	THR	CB-CA-C	5.31	120.48	109.38
1	F	196	THR	CB-CA-C	-5.28	104.12	111.41
1	K	412	GLU	N-CA-C	-5.27	105.61	111.36
1	J	198	LEU	N-CA-C	5.27	118.17	111.69
1	E	83	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	F	284	ALA	N-CA-C	-5.26	105.22	111.69
1	E	83	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	H	84	ALA	N-CA-C	5.25	116.69	111.07
1	L	156	GLU	CA-C-N	-5.24	114.52	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	156	GLU	C-N-CA	-5.24	114.52	119.76
1	F	202	TYR	N-CA-C	-5.23	105.66	111.36
1	H	187	THR	N-CA-C	-5.23	101.42	109.52
1	J	448	THR	N-CA-C	5.22	117.58	108.76
1	C	253	MET	CG-SD-CE	-5.21	89.43	100.90
1	I	274	ILE	N-CA-C	5.21	115.08	107.37
1	L	171	LEU	N-CA-C	5.21	116.76	111.14
1	B	135	THR	N-CA-CB	5.19	117.75	110.12
1	F	340	GLY	CA-C-N	5.18	125.19	120.21
1	F	340	GLY	C-N-CA	5.18	125.19	120.21
1	D	158	VAL	CA-CB-CG2	5.18	119.20	110.40
1	G	263	VAL	CA-C-N	-5.17	115.18	122.94
1	G	263	VAL	C-N-CA	-5.17	115.18	122.94
1	C	112	PRO	CA-C-N	5.16	127.44	120.38
1	C	112	PRO	C-N-CA	5.16	127.44	120.38
1	B	484	THR	N-CA-CB	-5.15	101.67	111.00
1	C	135	THR	CB-CA-C	-5.15	102.24	110.79
1	H	477	SER	CA-C-N	5.14	127.16	120.28
1	H	477	SER	C-N-CA	5.14	127.16	120.28
1	E	217	VAL	CG1-CB-CG2	5.14	122.10	110.80
1	D	110	GLY	N-CA-C	5.13	120.84	114.37
1	D	20	ILE	CB-CA-C	-5.13	104.74	111.25
1	E	246	THR	N-CA-C	5.12	116.86	111.28
1	F	423	TYR	N-CA-C	5.12	117.46	110.55
1	G	98	ARG	N-CA-C	5.12	117.25	111.11
1	E	124	THR	CA-CB-CG2	5.12	119.20	110.50
1	C	171	LEU	CB-CG-CD2	5.11	126.03	110.70
1	J	135	THR	N-CA-CB	5.09	118.06	110.22
1	K	47	VAL	N-CA-C	-5.09	102.06	108.93
1	L	59	ILE	CB-CA-C	-5.09	105.27	112.14
1	J	365	VAL	CB-CA-C	5.08	117.71	111.25
1	D	135	THR	N-CA-CB	5.08	117.68	110.06
1	J	484	THR	N-CA-CB	-5.08	102.13	111.37
1	L	27	GLU	N-CA-C	5.07	117.83	109.72
1	L	187	THR	N-CA-C	-5.07	101.03	108.99
1	F	274	ILE	N-CA-C	5.07	115.39	107.99
1	A	87	ILE	N-CA-C	5.07	115.79	110.62
1	F	59	ILE	CB-CA-C	-5.07	105.49	111.97
1	D	422	SER	CA-CB-OG	-5.06	100.98	111.10
1	A	115	VAL	N-CA-CB	5.05	119.00	110.56
1	H	484	THR	N-CA-CB	-5.05	102.05	110.83
1	A	443	LYS	N-CA-C	5.04	119.48	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	438	HIS	N-CA-C	5.04	116.58	111.14
1	C	187	THR	CA-CB-OG1	5.03	117.15	109.60
1	F	132	ALA	N-CA-C	-5.03	105.25	111.33
1	D	484	THR	N-CA-CB	-5.02	102.49	111.08
1	L	196	THR	N-CA-C	5.02	116.78	109.30
1	G	217	VAL	CB-CA-C	5.02	118.23	110.50
1	K	117	LEU	N-CA-C	5.01	116.44	110.97
1	L	181	ALA	N-CA-C	5.01	117.14	111.02
1	B	435	LYS	N-CA-C	5.01	116.55	111.14
1	F	188	ILE	N-CA-C	5.01	115.86	108.45
1	H	49	ALA	N-CA-C	5.01	116.42	108.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	493	ILE	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	3791	0	3743	61	0
1	B	3791	0	3743	57	0
1	C	3793	0	3742	53	0
1	D	3787	0	3742	54	0
1	E	3781	0	3731	55	0
1	F	3794	0	3748	76	0
1	G	3781	0	3731	76	0
1	H	3787	0	3737	76	0
1	I	3788	0	3738	69	0
1	J	3788	0	3738	68	0
1	K	3773	0	3725	84	0
1	L	3764	0	3714	92	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	255	0	0	11	0
3	B	123	0	0	3	0
3	C	197	0	0	3	0
3	D	216	0	0	5	0
3	E	218	0	0	1	0
3	F	124	0	0	2	0
3	G	152	0	0	4	0
3	H	143	0	0	3	0
3	I	109	0	0	1	0
3	J	74	0	0	4	0
3	K	76	0	0	3	0
3	L	62	0	0	4	0
All	All	47191	0	44832	739	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (739) 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:H:264:THR:CG2	1:H:264:THR:CB	1.75	1.63
1:G:264:THR:CB	1:G:264:THR:CG2	1.79	1.58
1:L:448:THR:HG23	3:L:627:HOH:O	1.60	1.02
1:D:88:TYR:CE2	3:D:689:HOH:O	2.12	1.01
1:I:173:MET:HE1	1:I:243:THR:HG21	1.42	0.98
1:L:32:ILE:HD12	1:L:58:ASP:OD1	1.70	0.91
1:F:127:ASN:HB3	3:F:716:HOH:O	1.69	0.91
1:L:327:VAL:HG11	1:L:381:PRO:HG2	1.53	0.89
1:J:357:GLN:O	1:J:361:GLU:HG3	1.73	0.88
1:F:235:HIS:HA	1:F:259:MET:HE3	1.55	0.87
1:G:243:THR:HB	1:G:266:GLU:HB2	1.57	0.86
1:D:235:HIS:HA	1:D:259:MET:HE3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LYS:HE2	3:A:740:HOH:O	1.77	0.84
1:C:9:LYS:H	1:C:103:GLN:HE22	1.25	0.83
1:C:66:ALA:HB1	1:C:187:THR:HG23	1.60	0.83
1:C:88:TYR:CD2	1:E:88:TYR:CZ	2.68	0.81
1:A:127:ASN:HB3	3:A:805:HOH:O	1.80	0.81
1:D:88:TYR:CD2	3:D:689:HOH:O	2.29	0.81
1:K:9:LYS:H	1:K:103:GLN:HE22	1.28	0.81
1:F:66:ALA:HB1	1:F:187:THR:HG22	1.60	0.81
1:H:243:THR:HG21	3:H:634:HOH:O	1.81	0.80
1:F:438:HIS:HE1	1:L:438:HIS:HE1	1.29	0.80
1:L:191:LYS:HG2	1:L:220:VAL:O	1.82	0.79
1:E:9:LYS:H	1:E:103:GLN:HE22	1.29	0.79
1:L:201:LEU:HD11	1:L:221:PRO:HG3	1.64	0.79
1:F:494:LYS:HG2	1:K:435:LYS:HE3	1.65	0.78
1:B:88:TYR:CD2	1:G:88:TYR:CE2	2.72	0.78
1:I:78:MET:HG2	1:I:82:GLU:HB2	1.63	0.78
1:D:127[A]:ASN:OD1	3:D:757:HOH:O	2.01	0.78
1:J:436:THR:HG21	3:J:671:HOH:O	1.81	0.78
1:B:88:TYR:CE2	1:G:88:TYR:CD2	2.73	0.77
1:F:188:ILE:HD13	1:F:190:LEU:HB2	1.66	0.77
1:G:243:THR:HG21	3:G:646:HOH:O	1.85	0.77
1:E:169:PHE:HB3	1:E:172:VAL:HG13	1.67	0.77
1:L:78:MET:HG2	1:L:82:GLU:HB2	1.66	0.76
1:C:494:LYS:HG3	1:E:435:LYS:HD3	1.67	0.76
1:F:243:THR:HB	1:F:266:GLU:HB2	1.67	0.76
1:H:9:LYS:H	1:H:103:GLN:HE22	1.32	0.76
1:A:438:HIS:HE1	1:E:438:HIS:HE1	1.33	0.76
1:A:88:TYR:CZ	1:D:88:TYR:CD2	2.74	0.75
1:K:433:ASN:HD22	1:K:436:THR:H	1.35	0.75
1:K:59:ILE:HD13	1:K:231:ILE:HG13	1.67	0.75
1:D:258:GLU:OE1	3:D:812:HOH:O	2.06	0.74
1:E:66:ALA:O	1:E:187:THR:HG21	1.86	0.74
1:K:66:ALA:O	1:K:187:THR:HG21	1.87	0.74
1:G:387:VAL:CG1	1:G:394:VAL:HG11	2.17	0.73
1:A:105:GLU:OE1	1:A:199[B]:SER:OG	2.05	0.73
1:B:9:LYS:H	1:B:103:GLN:HE22	1.34	0.73
1:F:374:GLU:HB2	1:F:375:LYS:CD	2.19	0.73
1:I:173:MET:CE	1:I:243:THR:HG21	2.16	0.73
1:G:126:GLU:HG2	3:G:708:HOH:O	1.88	0.73
1:A:9:LYS:H	1:A:103:GLN:HE22	1.37	0.73
1:H:88:TYR:CE2	1:I:88:TYR:CE2	2.77	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:LEU:HD13	1:H:333:MET:HG3	1.70	0.72
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.70	0.72
1:D:120:ASP:O	1:D:124:THR:HG23	1.88	0.72
1:L:26:GLY:HA3	1:L:214:ASN:HD22	1.55	0.72
1:C:88:TYR:CE2	1:E:88:TYR:CD2	2.78	0.72
1:E:66:ALA:HB1	1:E:187:THR:HG23	1.72	0.72
1:L:173:MET:HA	1:L:173:MET:HE2	1.71	0.72
1:G:245:SER:HG	1:G:248:THR:HG1	1.36	0.71
1:K:357:GLN:OE1	1:K:360:LYS:HE2	1.90	0.71
1:C:239:LYS:NZ	1:C:262:HIS:HD2	1.88	0.71
1:A:19:GLU:OE2	3:A:834:HOH:O	2.07	0.71
1:G:188:ILE:HD11	1:G:190:LEU:HB2	1.71	0.71
1:K:438:HIS:HD2	1:L:152:TYR:OH	1.72	0.71
1:D:9:LYS:H	1:D:103:GLN:HE22	1.38	0.70
1:B:438:HIS:HE1	1:H:438:HIS:HE1	1.40	0.70
1:C:66:ALA:O	1:C:187:THR:HG21	1.91	0.70
1:L:324:ALA:O	1:L:327:VAL:HG12	1.91	0.70
1:J:169:PHE:O	1:J:173:MET:HB2	1.91	0.69
1:L:191:LYS:HD3	1:L:192:PRO:O	1.91	0.69
1:C:88:TYR:CE2	1:E:88:TYR:CE2	2.80	0.69
1:G:78:MET:HG2	1:G:82:GLU:HB2	1.74	0.69
1:B:342:LEU:HD22	1:B:379:VAL:HG13	1.74	0.69
1:I:9:LYS:H	1:I:103:GLN:HE22	1.40	0.68
1:J:308:VAL:HG21	1:J:316:VAL:HG21	1.74	0.68
1:B:433:ASN:HD22	1:B:436:THR:H	1.41	0.68
1:A:120:ASP:O	1:A:124:THR:HG23	1.93	0.68
1:F:9:LYS:H	1:F:103:GLN:HE22	1.42	0.68
1:J:169:PHE:HB3	1:J:172:VAL:HG13	1.76	0.68
1:J:139:ILE:HD12	1:K:141:GLN:HG2	1.76	0.68
1:J:433:ASN:HB3	1:J:436:THR:HG23	1.76	0.68
1:A:264:THR:HB	3:A:730:HOH:O	1.94	0.67
1:G:438:HIS:HE1	1:I:438:HIS:HE1	1.41	0.67
1:L:433:ASN:HB3	1:L:436:THR:HG23	1.75	0.67
1:F:374:GLU:HB2	1:F:375:LYS:HD2	1.76	0.67
1:H:66:ALA:O	1:H:187:THR:HG21	1.95	0.67
1:K:12:VAL:HG11	1:K:103:GLN:HE21	1.58	0.67
1:J:433:ASN:HD22	1:J:436:THR:HG22	1.58	0.67
1:E:124:THR:HG21	1:E:171:LEU:HD13	1.77	0.66
1:L:66:ALA:O	1:L:187:THR:HG21	1.95	0.66
1:B:308:VAL:HG21	1:B:316:VAL:HG21	1.78	0.66
1:A:438:HIS:CE1	1:E:438:HIS:HE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASN:HD22	1:D:436:THR:H	1.44	0.66
1:L:243:THR:HB	1:L:266:GLU:HB2	1.77	0.66
1:A:88:TYR:CD1	3:A:821:HOH:O	2.48	0.66
1:D:107:LEU:HD13	1:D:333:MET:HG3	1.77	0.66
1:H:88:TYR:CZ	1:I:88:TYR:CD2	2.84	0.66
1:C:438:HIS:HE1	1:D:438:HIS:HE1	1.43	0.65
1:E:387:VAL:CG1	1:E:394:VAL:HG11	2.27	0.65
1:K:266:GLU:OE1	1:K:464:GLY:HA2	1.96	0.65
1:H:66:ALA:HB1	1:H:187:THR:HG23	1.78	0.65
1:K:254:ARG:HG2	1:L:254:ARG:HG3	1.78	0.65
1:I:364:THR:HG23	1:I:386:ASP:HB2	1.79	0.65
1:A:239:LYS:NZ	1:A:262:HIS:HD2	1.94	0.64
1:E:277:GLU:O	1:E:312:HIS:HE1	1.80	0.64
1:F:494:LYS:HG2	1:K:435:LYS:CE	2.28	0.64
1:A:88:TYR:CE2	1:D:88:TYR:CE2	2.85	0.64
1:J:356:GLU:O	1:J:360:LYS:HG2	1.98	0.64
1:H:243:THR:HB	1:H:266:GLU:HB2	1.79	0.64
1:A:277:GLU:OE2	1:A:311:LYS:HE3	1.98	0.64
1:B:438:HIS:CE1	1:H:438:HIS:HE1	2.15	0.64
1:F:438:HIS:CE1	1:L:438:HIS:HE1	2.13	0.64
1:B:448:THR:HG23	3:B:632:HOH:O	1.97	0.64
1:I:22:MET:HG3	1:I:221:PRO:HD2	1.80	0.64
1:E:120:ASP:O	1:E:124:THR:HG23	1.98	0.63
1:E:239:LYS:HZ3	1:E:262:HIS:HD2	1.45	0.63
1:F:188:ILE:HD12	1:F:188:ILE:C	2.23	0.63
1:H:120:ASP:O	1:H:124:THR:HG23	1.98	0.63
1:B:78:MET:HG2	1:B:82:GLU:HB2	1.80	0.63
1:J:259:MET:SD	1:J:261:LYS:HE3	2.38	0.63
1:C:88:TYR:CD2	1:E:88:TYR:CE2	2.86	0.62
1:A:88:TYR:CD2	1:D:88:TYR:CE2	2.87	0.62
1:L:239:LYS:HD2	1:L:482:ASN:O	2.00	0.62
1:A:260:ILE:HA	1:C:253:MET:HE1	1.81	0.62
1:E:239:LYS:NZ	1:E:262:HIS:HD2	1.97	0.62
1:H:239:LYS:HZ3	1:H:262:HIS:HD2	1.45	0.62
1:B:158:VAL:HG12	1:B:485:GLU:HG2	1.80	0.61
1:A:433:ASN:HD22	1:A:436:THR:H	1.46	0.61
1:C:239:LYS:HZ3	1:C:262:HIS:HD2	1.46	0.61
1:G:127:ASN:HB3	3:G:723:HOH:O	2.00	0.61
1:G:264:THR:CG2	1:G:264:THR:CA	2.77	0.61
1:J:387:VAL:HG13	1:J:394:VAL:HG21	1.82	0.61
1:H:436:THR:HG21	3:H:736:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:438:HIS:CD2	1:L:152:TYR:OH	2.52	0.61
1:F:374:GLU:HB2	1:F:375:LYS:HD3	1.82	0.61
1:F:374:GLU:CB	1:F:375:LYS:HD2	2.29	0.61
1:L:387:VAL:CG1	1:L:394:VAL:CG2	2.78	0.61
1:G:370:GLU:HG2	1:G:380:LYS:HD2	1.80	0.61
1:J:239:LYS:NZ	1:J:262:HIS:HD2	1.98	0.61
1:A:88:TYR:CE1	3:A:821:HOH:O	2.53	0.61
1:B:88:TYR:CE2	1:G:88:TYR:CE2	2.88	0.61
1:F:66:ALA:HB1	1:F:187:THR:CG2	2.30	0.61
1:J:178:MET:HG2	1:J:188:ILE:HD12	1.82	0.61
1:H:277:GLU:O	1:H:312:HIS:HE1	1.84	0.60
1:H:48:LEU:HD11	1:H:107:LEU:HB3	1.83	0.60
1:C:433:ASN:HD22	1:C:436:THR:H	1.49	0.60
1:I:126:GLU:HG3	3:I:690:HOH:O	2.01	0.60
1:G:387:VAL:HG11	1:G:404:VAL:HG11	1.83	0.60
1:H:264:THR:CG2	1:H:264:THR:CA	2.74	0.60
1:B:308:VAL:HG21	1:B:316:VAL:CG2	2.32	0.60
1:H:88:TYR:CD2	1:I:88:TYR:CE2	2.90	0.60
1:I:433:ASN:HD22	1:I:436:THR:H	1.48	0.60
1:F:124:THR:HG21	1:F:171:LEU:HD13	1.83	0.59
1:L:405:VAL:C	1:L:406:LEU:HD23	2.27	0.59
1:J:173:MET:HG3	3:J:646:HOH:O	2.02	0.59
1:J:387:VAL:HG13	1:J:394:VAL:CG2	2.32	0.59
1:D:190:LEU:HD12	1:D:200:LEU:HD21	1.85	0.59
1:H:239:LYS:NZ	1:H:262:HIS:HD2	2.01	0.59
1:I:78:MET:HG2	1:I:82:GLU:CB	2.32	0.59
1:K:105:GLU:OE1	1:K:199:SER:HB3	2.02	0.59
1:F:447:GLY:HA3	1:F:464:GLY:O	2.02	0.59
1:J:9:LYS:H	1:J:103:GLN:HE22	1.48	0.59
1:D:364:THR:CG2	1:D:386:ASP:OD2	2.51	0.59
1:F:88:TYR:CD2	1:K:88:TYR:CZ	2.91	0.59
1:F:163:GLN:HB2	1:F:190:LEU:HD23	1.85	0.59
1:L:163:GLN:HB2	1:L:190:LEU:HD23	1.84	0.59
1:L:239:LYS:HZ3	1:L:264:THR:HG23	1.67	0.59
1:L:78:MET:HG2	1:L:82:GLU:CB	2.32	0.58
1:L:277:GLU:O	1:L:312:HIS:HE1	1.87	0.58
1:B:492:ASN:C	1:B:492:ASN:HD22	2.11	0.58
1:I:120:ASP:O	1:I:124:THR:HG23	2.03	0.58
1:C:239:LYS:NZ	1:C:262:HIS:CD2	2.71	0.58
1:F:84:ALA:HB2	1:F:135:THR:OG1	2.03	0.58
1:K:260:ILE:HD12	1:L:468:GLN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ARG:O	1:D:71:GLU:HG3	2.03	0.58
1:G:163:GLN:OE1	1:G:188:ILE:CD1	2.51	0.57
1:L:239:LYS:NZ	1:L:264:THR:HG23	2.19	0.57
1:D:239:LYS:HZ3	1:D:262:HIS:HD2	1.53	0.57
1:L:447:GLY:HA3	1:L:464:GLY:O	2.05	0.57
1:D:239:LYS:NZ	1:D:262:HIS:HD2	2.02	0.57
1:G:178:MET:HG2	1:G:188:ILE:HD13	1.86	0.57
1:H:433:ASN:HD22	1:H:436:THR:H	1.52	0.57
1:J:492:ASN:ND2	1:J:494:LYS:H	2.02	0.57
1:F:158:VAL:HG12	1:F:485:GLU:HG2	1.87	0.57
1:H:84:ALA:HB2	1:H:135:THR:OG1	2.04	0.57
1:B:120:ASP:O	1:B:124:THR:HG23	2.04	0.57
1:K:19:GLU:OE1	3:K:638:HOH:O	2.17	0.57
1:H:391:MET:HB2	1:H:394:VAL:CG1	2.35	0.56
1:L:387:VAL:CG1	1:L:394:VAL:HG21	2.35	0.56
1:A:239:LYS:HZ1	1:A:264:THR:HG22	1.69	0.56
1:A:492:ASN:HD22	1:A:492:ASN:C	2.13	0.56
1:G:239:LYS:NZ	1:G:262:HIS:HD2	2.02	0.56
1:L:22:MET:HE3	1:L:24:ILE:CD1	2.35	0.56
1:G:88:TYR:CE1	1:G:129:ARG:HG2	2.41	0.56
1:G:112:PRO:HB2	1:G:115:VAL:HG13	1.87	0.56
1:H:350:ARG:NH1	3:H:664:HOH:O	2.29	0.56
1:K:66:ALA:HB1	1:K:187:THR:HG23	1.86	0.56
1:F:492:ASN:HD22	1:F:492:ASN:C	2.14	0.56
1:H:371:ARG:HD3	1:H:372:ALA:N	2.20	0.56
1:J:364:THR:HG23	1:J:386:ASP:HB2	1.87	0.56
1:G:357:GLN:HE22	1:G:360:LYS:HE3	1.71	0.56
1:B:124:THR:HG22	1:B:172:VAL:HA	1.87	0.56
1:B:239:LYS:NZ	1:B:262:HIS:HD2	2.03	0.56
1:I:374:GLU:HB2	1:I:375:LYS:HE3	1.88	0.56
1:L:26:GLY:HA3	1:L:214:ASN:ND2	2.20	0.56
1:C:494:LYS:HG3	1:E:435:LYS:CD	2.36	0.55
1:F:194:SER:OG	1:F:223:PHE:CE1	2.54	0.55
1:D:22:MET:CG	1:D:221:PRO:HD2	2.36	0.55
1:J:433:ASN:HD22	1:J:436:THR:CG2	2.18	0.55
1:G:191:LYS:HG2	1:G:220:VAL:O	2.07	0.55
1:I:112:PRO:HB2	1:I:115:VAL:HG13	1.86	0.55
1:G:9:LYS:H	1:G:103:GLN:HE22	1.52	0.55
1:J:78:MET:SD	1:J:83:ARG:HG2	2.47	0.55
1:L:492:ASN:C	1:L:492:ASN:HD22	2.15	0.55
1:C:124:THR:HG21	1:C:171:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:TRP:CZ2	1:F:83:ARG:HD2	2.42	0.55
1:G:438:HIS:HE1	1:I:438:HIS:CE1	2.25	0.55
1:A:484:THR:HG22	3:A:657:HOH:O	2.05	0.55
1:C:361:GLU:OE1	3:C:717:HOH:O	2.18	0.55
1:G:239:LYS:HZ3	1:G:262:HIS:HD2	1.53	0.55
1:C:364:THR:HG23	1:C:386:ASP:HB2	1.89	0.55
1:C:78:MET:HG3	1:C:82:GLU:HB2	1.90	0.54
1:E:9:LYS:H	1:E:103:GLN:NE2	2.03	0.54
1:G:387:VAL:CG1	1:G:394:VAL:CG1	2.85	0.54
1:G:176:TRP:CZ2	1:G:475:LEU:HD11	2.42	0.54
1:H:177:LYS:HZ1	1:H:243:THR:HG22	1.72	0.54
1:C:438:HIS:CE1	1:D:438:HIS:HE1	2.26	0.54
1:K:70:PHE:CZ	1:K:159:GLY:HA2	2.42	0.54
1:G:433:ASN:HD22	1:G:436:THR:H	1.55	0.54
1:H:169:PHE:HB3	1:H:172:VAL:HG22	1.90	0.54
1:J:438:HIS:CE1	1:K:438:HIS:HE1	2.25	0.54
1:F:282:GLU:HA	1:F:282:GLU:OE2	2.07	0.54
1:G:84:ALA:HB2	1:G:135:THR:OG1	2.08	0.54
1:K:26:GLY:HA3	1:K:214:ASN:ND2	2.23	0.54
1:C:48:LEU:HD11	1:C:107:LEU:HB3	1.90	0.54
1:C:492:ASN:C	1:C:492:ASN:HD22	2.15	0.54
1:F:177:LYS:HZ1	1:F:243:THR:HG22	1.73	0.53
1:G:260:ILE:HA	1:H:253:MET:HE1	1.91	0.53
1:A:76:ALA:O	1:E:147:LYS:HD3	2.09	0.53
1:K:285:ILE:HG12	1:K:316:VAL:HB	1.89	0.53
1:C:9:LYS:H	1:C:103:GLN:NE2	1.99	0.53
1:K:84:ALA:HB2	1:K:135:THR:OG1	2.08	0.53
1:L:8:LEU:HA	1:L:103:GLN:HE22	1.73	0.53
1:A:290:GLN:CG	3:A:850:HOH:O	2.57	0.53
1:B:239:LYS:HZ3	1:B:262:HIS:HD2	1.57	0.53
1:D:492:ASN:C	1:D:492:ASN:HD22	2.16	0.53
1:F:492:ASN:ND2	1:F:494:LYS:H	2.07	0.53
1:L:191:LYS:CG	1:L:220:VAL:O	2.57	0.53
1:C:494:LYS:HE3	1:E:439:GLN:OE1	2.09	0.53
1:F:9:LYS:H	1:F:103:GLN:NE2	2.07	0.53
1:J:448:THR:CG2	3:J:669:HOH:O	2.55	0.53
1:K:364:THR:CG2	1:K:386:ASP:OD2	2.57	0.53
1:E:59:ILE:HD12	1:E:231:ILE:CG1	2.38	0.52
1:I:48:LEU:HD11	1:I:107:LEU:HB3	1.90	0.52
1:I:239:LYS:HZ3	1:I:262:HIS:HD2	1.57	0.52
1:F:438:HIS:HD2	1:J:152:TYR:OH	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:LYS:O	1:F:350:ARG:HG3	2.09	0.52
1:D:364:THR:HG23	1:D:386:ASP:OD2	2.09	0.52
1:E:107:LEU:HD13	1:E:333:MET:HG3	1.91	0.52
1:A:78:MET:HG2	1:A:82:GLU:HB2	1.92	0.52
1:A:239:LYS:HZ1	1:A:264:THR:CG2	2.22	0.52
1:E:387:VAL:HG13	1:E:394:VAL:CG1	2.40	0.52
1:F:433:ASN:HD22	1:F:436:THR:H	1.57	0.52
1:G:253:MET:HG3	1:G:265:LEU:HD11	1.90	0.52
1:I:107:LEU:HD13	1:I:333:MET:HG3	1.92	0.52
1:K:59:ILE:HD12	1:K:230:ALA:HB3	1.92	0.52
1:A:88:TYR:CE2	1:D:88:TYR:CD2	2.97	0.52
1:C:415:ILE:HD13	1:C:443:LYS:HD2	1.91	0.52
1:I:163:GLN:HB2	1:I:190:LEU:HD23	1.92	0.52
1:I:190:LEU:HD12	1:I:200:LEU:HD21	1.92	0.52
1:K:364:THR:HG21	1:K:386:ASP:OD2	2.09	0.52
1:L:22:MET:HE3	1:L:24:ILE:HD11	1.91	0.52
1:E:492:ASN:C	1:E:492:ASN:HD22	2.17	0.52
1:G:124:THR:HG21	1:G:171:LEU:HD13	1.91	0.52
1:B:387:VAL:HG13	1:B:394:VAL:HG11	1.91	0.52
1:E:188:ILE:CD1	1:E:190:LEU:HB2	2.39	0.52
1:B:48:LEU:HD11	1:B:107:LEU:HB3	1.92	0.52
1:C:84:ALA:HB2	1:C:135:THR:OG1	2.09	0.52
1:D:190:LEU:HD12	1:D:200:LEU:CD2	2.39	0.52
1:E:387:VAL:CG1	1:E:394:VAL:CG1	2.88	0.51
1:I:166:PRO:HD3	1:I:243:THR:HB	1.91	0.51
1:L:251:TYR:O	1:L:255:GLN:HG2	2.10	0.51
1:I:105:GLU:OE1	1:I:105:GLU:HA	2.10	0.51
1:K:188:ILE:CD1	1:K:190:LEU:HB2	2.41	0.51
1:E:492:ASN:ND2	1:E:494:LYS:H	2.09	0.51
1:J:438:HIS:HE1	1:K:438:HIS:HE1	1.58	0.51
1:K:12:VAL:HG11	1:K:103:GLN:NE2	2.24	0.51
1:F:88:TYR:CE2	1:K:88:TYR:CE2	2.99	0.51
1:G:357:GLN:HE22	1:G:360:LYS:CE	2.23	0.51
1:J:107:LEU:HD13	1:J:333:MET:HG3	1.92	0.51
1:J:329:LEU:HD12	1:J:339:MET:HB3	1.91	0.51
1:F:438:HIS:HE1	1:L:438:HIS:CE1	2.19	0.51
1:H:387:VAL:CG1	1:H:394:VAL:HG11	2.40	0.51
1:A:277:GLU:OE2	1:A:311:LYS:CE	2.57	0.51
1:E:387:VAL:HG13	1:E:394:VAL:HG11	1.92	0.51
1:I:243:THR:HG23	1:I:266:GLU:HB3	1.92	0.51
1:K:492:ASN:ND2	1:K:494:LYS:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:HD22	1:B:379:VAL:CG1	2.39	0.51
1:D:163:GLN:HB2	1:D:190:LEU:HD23	1.92	0.51
1:D:364:THR:HG23	1:D:386:ASP:HB2	1.93	0.51
1:G:438:HIS:CE1	1:I:438:HIS:HE1	2.24	0.51
1:K:372:ALA:HB2	1:K:380:LYS:HG3	1.93	0.51
1:L:239:LYS:NZ	1:L:262:HIS:HD2	2.08	0.51
1:B:99:GLU:O	1:B:103:GLN:HG3	2.10	0.51
1:H:387:VAL:CG1	1:H:394:VAL:CG1	2.89	0.51
1:K:254:ARG:HG2	1:L:254:ARG:CG	2.40	0.51
1:L:327:VAL:HG13	1:L:327:VAL:O	2.10	0.51
1:B:22:MET:CG	1:B:221:PRO:HD2	2.41	0.51
1:E:364:THR:CG2	1:E:386:ASP:OD2	2.59	0.51
1:F:188:ILE:CD1	1:F:190:LEU:HB2	2.38	0.51
1:H:388:THR:O	1:H:394:VAL:HG11	2.11	0.51
1:I:84:ALA:HB2	1:I:135:THR:OG1	2.11	0.51
1:I:239:LYS:NZ	1:I:262:HIS:HD2	2.08	0.51
1:B:78:MET:SD	1:B:83:ARG:HG2	2.51	0.50
1:L:9:LYS:H	1:L:103:GLN:HE22	1.57	0.50
1:L:66:ALA:HB1	1:L:187:THR:HG23	1.93	0.50
1:G:152:TYR:OH	1:H:438:HIS:HD2	1.94	0.50
1:L:235:HIS:HA	1:L:259:MET:SD	2.51	0.50
1:D:253:MET:HG3	1:D:265:LEU:HD11	1.93	0.50
1:E:59:ILE:CD1	1:E:220:VAL:HG21	2.42	0.50
1:J:149:TYR:CD1	1:J:492:ASN:HA	2.46	0.50
1:K:26:GLY:HA3	1:K:214:ASN:HD22	1.77	0.50
1:K:67:ARG:O	1:K:71:GLU:HG2	2.10	0.50
1:B:484:THR:HG21	3:B:635:HOH:O	2.11	0.50
1:D:18:GLU:HG3	3:D:711:HOH:O	2.12	0.50
1:F:312:HIS:O	1:F:316:VAL:HG13	2.11	0.50
1:H:253:MET:HE2	1:H:265:LEU:HD11	1.93	0.50
1:I:415:ILE:HD13	1:I:443:LYS:HD2	1.93	0.50
1:K:21:LYS:HE2	1:K:29:VAL:HA	1.92	0.50
1:I:374:GLU:HB2	1:I:375:LYS:CE	2.41	0.50
1:A:112:PRO:HB2	1:A:115:VAL:HG13	1.94	0.50
1:A:178:MET:HG2	1:A:188:ILE:HD13	1.94	0.50
1:F:112:PRO:HB2	1:F:115:VAL:HG13	1.94	0.50
1:B:148:ASP:HB3	1:B:494:LYS:HG3	1.93	0.50
1:K:120:ASP:O	1:K:124:THR:HG23	2.11	0.50
1:L:254:ARG:O	1:L:257:ALA:HB3	2.12	0.50
1:G:163:GLN:OE1	1:G:188:ILE:HD12	2.12	0.50
1:H:120:ASP:O	1:H:124:THR:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:PHE:HB3	1:G:172:VAL:HG13	1.94	0.50
1:J:239:LYS:HZ3	1:J:262:HIS:HD2	1.57	0.50
1:K:178:MET:HG2	1:K:188:ILE:HD13	1.93	0.50
1:E:201:LEU:HD11	1:E:221:PRO:HG3	1.93	0.49
1:J:9:LYS:HB2	1:J:12:VAL:HG13	1.94	0.49
1:B:438:HIS:HD2	1:I:152:TYR:OH	1.95	0.49
1:F:235:HIS:HA	1:F:259:MET:CE	2.33	0.49
1:G:153:THR:HA	1:G:487:LYS:O	2.12	0.49
1:G:78:MET:SD	1:G:83:ARG:HG2	2.52	0.49
1:H:264:THR:CG2	1:H:264:THR:HA	2.41	0.49
1:H:364:THR:CG2	1:H:386:ASP:OD2	2.60	0.49
1:B:84:ALA:HB2	1:B:135:THR:OG1	2.13	0.49
1:H:124:THR:HG21	1:H:171:LEU:HD13	1.94	0.49
1:J:190:LEU:HD12	1:J:200:LEU:CD2	2.42	0.49
1:K:85:HIS:CE1	1:K:89:LYS:HE2	2.47	0.49
1:K:433:ASN:HD21	1:K:435:LYS:HB2	1.78	0.49
1:E:253:MET:HE2	1:E:265:LEU:HD11	1.92	0.49
1:I:158:VAL:HG23	1:I:483:TYR:C	2.37	0.49
1:K:391:MET:HB2	1:K:394:VAL:HG13	1.94	0.49
1:K:98:ARG:CZ	1:K:117:LEU:HD11	2.43	0.49
1:L:327:VAL:HG11	1:L:381:PRO:CG	2.36	0.49
1:C:447:GLY:HA3	1:C:464:GLY:O	2.12	0.49
1:J:161:VAL:O	1:J:161:VAL:HG13	2.12	0.49
1:J:492:ASN:C	1:J:492:ASN:HD22	2.19	0.49
1:K:327:VAL:HG22	1:K:329:LEU:CD2	2.43	0.49
1:C:372:ALA:HB2	1:C:380:LYS:HG3	1.95	0.49
1:G:391:MET:HB2	1:G:394:VAL:HG13	1.95	0.49
1:F:317:VAL:HG22	1:F:405:VAL:HG11	1.95	0.49
1:L:464:GLY:HA3	1:L:473:ARG:HD3	1.94	0.49
1:B:9:LYS:H	1:B:103:GLN:NE2	2.06	0.49
1:H:177:LYS:HZ1	1:H:243:THR:CG2	2.24	0.49
1:K:289:PHE:CG	1:K:323:MET:HE2	2.48	0.49
1:L:387:VAL:HG11	1:L:394:VAL:CG2	2.42	0.49
1:I:163:GLN:CB	1:I:190:LEU:HD23	2.42	0.48
1:A:35:LYS:HG3	3:A:696:HOH:O	2.13	0.48
1:E:59:ILE:HD12	1:E:231:ILE:HG12	1.95	0.48
1:G:277:GLU:O	1:G:312:HIS:HE1	1.95	0.48
1:G:471:ILE:HG13	1:H:260:ILE:HG22	1.95	0.48
1:H:92:ASP:O	1:H:96:GLU:HG3	2.13	0.48
1:I:156:GLU:O	1:I:484:THR:HA	2.13	0.48
1:J:161:VAL:HG12	1:J:187:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:161:VAL:HG21	1:K:483:TYR:CE1	2.48	0.48
1:L:493:ILE:O	1:L:494:LYS:HB2	2.13	0.48
1:B:178:MET:HG2	1:B:188:ILE:HD13	1.94	0.48
1:F:22:MET:HE1	1:F:31:ALA:HB2	1.95	0.48
1:F:260:ILE:HA	1:J:253:MET:HE1	1.94	0.48
1:G:107:LEU:HD13	1:G:333:MET:HG3	1.94	0.48
1:I:191:LYS:HG2	1:I:220:VAL:O	2.13	0.48
1:F:35:LYS:HB2	3:F:701:HOH:O	2.12	0.48
1:B:372:ALA:HB2	1:B:380:LYS:HG3	1.95	0.48
1:G:78:MET:HG2	1:G:82:GLU:CB	2.42	0.48
1:H:387:VAL:HG12	1:H:394:VAL:HG11	1.96	0.48
1:J:190:LEU:HD12	1:J:200:LEU:HD21	1.95	0.48
1:K:433:ASN:ND2	1:K:436:THR:HG23	2.28	0.48
1:E:350:ARG:HD3	3:E:657:HOH:O	2.13	0.48
1:H:59:ILE:HG13	1:H:230:ALA:HB3	1.95	0.48
1:K:357:GLN:O	1:K:361:GLU:HB2	2.14	0.48
1:L:290:GLN:HB3	3:L:613:HOH:O	2.13	0.48
1:B:190:LEU:CD1	1:B:200:LEU:CD2	2.92	0.48
1:C:239:LYS:HZ1	1:C:262:HIS:CD2	2.31	0.48
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.96	0.48
1:F:296:HIS:CD2	1:F:296:HIS:N	2.81	0.48
1:H:9:LYS:H	1:H:103:GLN:NE2	2.08	0.48
1:J:165:ILE:HG22	1:J:177:LYS:HE2	1.96	0.48
1:A:21:LYS:NZ	3:A:834:HOH:O	2.22	0.48
1:A:123:ALA:O	1:A:127:ASN:CG	2.56	0.48
1:C:165:ILE:HB	1:C:166:PRO:HD2	1.96	0.48
1:D:22:MET:HG3	1:D:221:PRO:HD2	1.95	0.48
1:G:177:LYS:NZ	1:G:243:THR:CG2	2.77	0.48
1:K:492:ASN:HD22	1:K:492:ASN:C	2.21	0.48
1:B:391:MET:HB2	1:B:394:VAL:HG13	1.94	0.48
1:B:438:HIS:HE1	1:H:438:HIS:CE1	2.26	0.48
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.95	0.48
1:H:328:LYS:HE3	1:H:336:GLU:HB3	1.96	0.48
1:K:112:PRO:HB2	1:K:115:VAL:HG13	1.94	0.47
1:K:246:THR:HG22	1:K:250:LYS:HE3	1.96	0.47
1:K:325:ASN:HD21	1:K:367:ALA:HB1	1.78	0.47
1:L:194:SER:HB3	1:L:222:GLY:O	2.14	0.47
1:C:78:MET:HG3	1:C:82:GLU:CB	2.43	0.47
1:C:88:TYR:CZ	1:C:129:ARG:HG2	2.49	0.47
1:D:103:GLN:O	1:D:107:LEU:HD22	2.14	0.47
1:F:142:THR:OG1	1:L:140:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:75:TRP:CH2	1:K:83:ARG:HG3	2.49	0.47
1:A:78:MET:SD	1:A:83:ARG:HG2	2.54	0.47
1:D:78:MET:HG2	1:D:82:GLU:CB	2.45	0.47
1:I:451:ILE:O	1:I:452:ASN:HB2	2.14	0.47
1:K:351:VAL:CG2	1:K:379:VAL:HG21	2.45	0.47
1:F:280:ASP:HB2	1:F:432:GLN:OE1	2.15	0.47
1:I:277:GLU:O	1:I:312:HIS:HE1	1.96	0.47
1:A:253:MET:HE2	1:A:265:LEU:HD11	1.96	0.47
1:E:59:ILE:HD11	1:E:220:VAL:HG21	1.95	0.47
1:F:99:GLU:O	1:F:103:GLN:HG3	2.14	0.47
1:G:190:LEU:C	1:G:190:LEU:HD23	2.39	0.47
1:I:9:LYS:H	1:I:103:GLN:NE2	2.09	0.47
1:C:9:LYS:N	1:C:103:GLN:HE22	2.02	0.47
1:F:438:HIS:CE1	1:L:438:HIS:CE1	3.00	0.47
1:G:188:ILE:CD1	1:G:190:LEU:HB2	2.43	0.47
1:G:357:GLN:NE2	1:G:360:LYS:HE3	2.29	0.47
1:H:135:THR:HG22	1:H:183:ALA:HA	1.95	0.47
1:I:135:THR:HG22	1:I:183:ALA:HA	1.96	0.47
1:B:492:ASN:HD21	1:B:494:LYS:HB2	1.79	0.47
1:D:364:THR:HG21	1:D:386:ASP:OD2	2.14	0.47
1:F:88:TYR:CE2	1:K:88:TYR:CD2	3.03	0.47
1:L:78:MET:SD	1:L:83:ARG:HG2	2.54	0.47
1:L:163:GLN:CB	1:L:190:LEU:HD23	2.43	0.47
1:B:78:MET:HG2	1:B:82:GLU:CB	2.45	0.47
1:C:438:HIS:HE1	1:D:438:HIS:CE1	2.27	0.47
1:F:147:LYS:HD2	1:L:76:ALA:O	2.14	0.47
1:G:387:VAL:HG11	1:G:394:VAL:CG1	2.45	0.47
1:I:296:HIS:N	1:I:296:HIS:CD2	2.83	0.47
1:J:448:THR:HG23	3:J:669:HOH:O	2.15	0.47
1:J:173:MET:CE	1:J:173:MET:HA	2.45	0.47
1:E:391:MET:HB2	1:E:394:VAL:HG13	1.97	0.47
1:K:43:ALA:HB2	3:K:642:HOH:O	2.14	0.47
1:K:172:VAL:HG13	3:K:641:HOH:O	2.15	0.47
1:A:8:LEU:HB3	1:A:13:GLU:OE2	2.15	0.46
1:F:493:ILE:HA	1:K:435:LYS:HG3	1.96	0.46
1:I:364:THR:HG21	1:I:386:ASP:OD2	2.15	0.46
1:L:134:TRP:O	1:L:138:ILE:HG13	2.15	0.46
1:A:290:GLN:HG3	3:A:850:HOH:O	2.13	0.46
1:D:235:HIS:CA	1:D:259:MET:HE3	2.38	0.46
1:H:88:TYR:CD2	1:I:88:TYR:CZ	3.04	0.46
1:H:163:GLN:OE1	1:H:188:ILE:HD13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:347:GLN:O	1:J:351:VAL:HG13	2.14	0.46
1:L:228:GLY:O	1:L:232:VAL:HG12	2.15	0.46
1:A:439:GLN:HE22	1:D:494:LYS:HE3	1.80	0.46
1:E:9:LYS:CE	1:E:99:GLU:OE2	2.62	0.46
1:A:277:GLU:O	1:A:312:HIS:HE1	1.99	0.46
1:C:75:TRP:CH2	1:C:83:ARG:HG3	2.51	0.46
1:G:19:GLU:OE1	3:G:743:HOH:O	2.21	0.46
1:H:259:MET:O	1:H:260:ILE:C	2.57	0.46
1:A:239:LYS:HZ3	1:A:262:HIS:HD2	1.61	0.46
1:C:239:LYS:HE2	1:C:482:ASN:O	2.16	0.46
1:D:9:LYS:H	1:D:103:GLN:NE2	2.09	0.46
1:H:67:ARG:O	1:H:71:GLU:HG3	2.15	0.46
1:I:124:THR:HG21	1:I:171:LEU:HB3	1.98	0.46
1:L:153:THR:HA	1:L:487:LYS:O	2.15	0.46
1:B:207:PHE:CD2	1:B:217:VAL:HG11	2.50	0.46
1:H:296:HIS:N	1:H:296:HIS:CD2	2.84	0.46
1:C:126:GLU:HG3	3:C:731:HOH:O	2.15	0.46
1:K:242:PHE:CZ	1:K:248:THR:HB	2.50	0.46
1:L:9:LYS:NZ	1:L:99:GLU:OE2	2.47	0.46
1:C:434:ILE:HB	1:D:434:ILE:HA	1.98	0.46
1:F:163:GLN:CD	1:F:177:LYS:HB3	2.40	0.46
1:I:272:PRO:HG3	1:I:418:ALA:HB1	1.98	0.46
1:J:48:LEU:HD11	1:J:107:LEU:HB3	1.98	0.46
1:J:296:HIS:N	1:J:296:HIS:CD2	2.84	0.46
1:H:124:THR:HG22	1:H:172:VAL:HG12	1.97	0.45
1:H:149:TYR:CD1	1:H:492:ASN:HA	2.51	0.45
1:A:124:THR:HG22	1:A:172:VAL:HA	1.98	0.45
1:A:308:VAL:HG11	1:A:316:VAL:HG13	1.97	0.45
1:E:188:ILE:HG12	1:E:217:VAL:HG22	1.98	0.45
1:F:75:TRP:CH2	1:F:83:ARG:HD2	2.51	0.45
1:H:75:TRP:CZ3	1:H:83:ARG:HG2	2.51	0.45
1:J:59:ILE:HD12	1:J:220:VAL:HG21	1.99	0.45
1:K:9:LYS:H	1:K:103:GLN:NE2	2.04	0.45
1:B:296:HIS:ND1	1:B:341:PRO:O	2.47	0.45
1:H:88:TYR:CG	1:I:88:TYR:CZ	3.05	0.45
1:B:152:TYR:OH	1:I:438:HIS:HD2	1.99	0.45
1:H:364:THR:HG23	1:H:386:ASP:OD2	2.16	0.45
1:K:188:ILE:HD12	1:K:190:LEU:HB2	1.98	0.45
1:L:342:LEU:CD2	1:L:351:VAL:HG21	2.46	0.45
1:F:44:THR:O	1:F:45:GLU:HB2	2.17	0.45
1:K:158:VAL:HG23	1:K:483:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:433:ASN:ND2	1:H:436:THR:HG23	2.31	0.45
1:J:166:PRO:HD2	1:J:173:MET:HG2	1.98	0.45
1:J:433:ASN:ND2	1:J:436:THR:HG22	2.28	0.45
1:L:254:ARG:NH1	1:L:255:GLN:OE1	2.49	0.45
1:C:492:ASN:ND2	1:C:494:LYS:H	2.14	0.45
1:G:188:ILE:HD11	1:G:190:LEU:HD12	1.98	0.45
1:G:492:ASN:C	1:G:492:ASN:HD22	2.25	0.45
1:H:85:HIS:HD2	1:I:88:TYR:OH	1.99	0.45
1:B:139:ILE:HD12	1:H:141:GLN:HG2	1.99	0.45
1:C:127:ASN:OD1	1:C:459:ALA:HB2	2.16	0.45
1:D:120:ASP:O	1:D:124:THR:CG2	2.61	0.45
1:J:433:ASN:HD21	1:J:435:LYS:HB2	1.82	0.45
1:K:188:ILE:HG12	1:K:217:VAL:HG22	1.99	0.45
1:A:38:GLU:OE2	1:G:35:LYS:NZ	2.50	0.45
1:A:239:LYS:HZ1	1:A:262:HIS:HD2	1.62	0.45
1:F:138:ILE:HG12	1:F:480:LEU:HD13	1.99	0.45
1:J:387:VAL:CG1	1:J:394:VAL:CG2	2.95	0.45
1:L:158:VAL:HG22	1:L:483:TYR:O	2.16	0.45
1:C:67:ARG:O	1:C:71:GLU:HG3	2.17	0.45
1:E:190:LEU:HD12	1:E:200:LEU:CD2	2.47	0.45
1:F:66:ALA:HA	1:F:187:THR:HG21	1.98	0.45
1:G:245:SER:OG	1:G:248:THR:OG1	2.08	0.45
1:G:264:THR:CG2	1:G:264:THR:OG1	2.54	0.45
1:B:239:LYS:HE2	1:B:482:ASN:O	2.18	0.44
1:D:161:VAL:HG22	1:D:188:ILE:HD13	1.98	0.44
1:G:177:LYS:NZ	1:G:474:GLU:OE2	2.49	0.44
1:H:201:LEU:HD11	1:H:221:PRO:HG3	1.99	0.44
1:I:447:GLY:HA3	1:I:464:GLY:O	2.17	0.44
1:E:364:THR:HG23	1:E:386:ASP:HB2	1.99	0.44
1:F:239:LYS:NZ	1:F:262:HIS:HD2	2.15	0.44
1:H:78:MET:HG2	1:H:82:GLU:HB2	2.00	0.44
1:H:245:SER:OG	1:H:248:THR:HG23	2.17	0.44
1:J:387:VAL:CG1	1:J:394:VAL:HG21	2.46	0.44
1:I:296:HIS:CD2	1:I:339:MET:HG3	2.52	0.44
1:I:464:GLY:HA3	1:I:473:ARG:HD3	1.98	0.44
1:A:239:LYS:HE2	1:A:482:ASN:O	2.18	0.44
1:D:78:MET:HG2	1:D:82:GLU:HB2	2.00	0.44
1:L:123:ALA:O	1:L:127:ASN:CG	2.61	0.44
1:L:191:LYS:HA	1:L:192:PRO:HD2	1.88	0.44
1:A:152:TYR:OH	1:C:438:HIS:HD2	2.01	0.44
1:I:173:MET:HE1	1:I:243:THR:CG2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:LEU:HA	1:F:103:GLN:HE22	1.81	0.44
1:K:217:VAL:HG13	1:K:219:PHE:CZ	2.53	0.44
1:L:190:LEU:HD22	1:L:191:LYS:N	2.33	0.44
1:L:484:THR:HG22	3:L:659:HOH:O	2.17	0.44
1:A:201:LEU:HD11	1:A:221:PRO:HG3	2.00	0.44
1:F:66:ALA:CA	1:F:187:THR:HG21	2.47	0.44
1:J:173:MET:HA	1:J:173:MET:HE3	1.99	0.44
1:L:296:HIS:CD2	1:L:296:HIS:N	2.86	0.44
1:L:364:THR:CG2	1:L:386:ASP:OD2	2.65	0.44
1:A:438:HIS:HD2	1:C:152:TYR:OH	2.01	0.44
1:H:78:MET:SD	1:H:83:ARG:HG3	2.57	0.44
1:J:48:LEU:HD13	1:J:198:LEU:CD1	2.48	0.44
1:L:145:ILE:HD12	1:L:151:ASN:CG	2.42	0.44
1:L:158:VAL:HG13	1:L:485:GLU:HG2	1.99	0.44
1:F:78:MET:HG2	1:F:82:GLU:HB3	2.00	0.44
1:F:88:TYR:CZ	1:K:88:TYR:CG	3.06	0.44
1:G:74:PRO:O	1:G:78:MET:HB2	2.18	0.44
1:H:292:ILE:HG12	1:H:403:VAL:HB	2.00	0.44
1:J:328:LYS:HE3	1:J:336:GLU:HB3	1.99	0.44
1:C:190:LEU:HD12	1:C:200:LEU:CD2	2.48	0.43
1:J:239:LYS:HE2	1:J:482:ASN:O	2.18	0.43
1:K:67:ARG:O	1:K:71:GLU:CG	2.66	0.43
1:L:351:VAL:CG2	1:L:379:VAL:HG21	2.47	0.43
1:D:331:ALA:HB3	1:D:334:GLU:CD	2.43	0.43
1:I:190:LEU:HD12	1:I:200:LEU:CD2	2.48	0.43
1:J:251:TYR:O	1:J:255:GLN:HG2	2.17	0.43
1:K:277:GLU:OE2	1:K:311:LYS:NZ	2.36	0.43
1:G:264:THR:CG2	1:G:264:THR:HA	2.47	0.43
1:H:88:TYR:CE2	1:I:88:TYR:CD2	3.05	0.43
1:K:326:ASN:HD22	1:K:326:ASN:HA	1.60	0.43
1:K:364:THR:HG23	1:K:386:ASP:HB2	2.00	0.43
1:L:41:ASN:C	1:L:41:ASN:OD1	2.60	0.43
1:A:134:TRP:O	1:A:138:ILE:HG13	2.19	0.43
1:B:447:GLY:HA3	1:B:464:GLY:O	2.18	0.43
1:A:239:LYS:HZ1	1:A:262:HIS:CD2	2.35	0.43
1:B:190:LEU:CD1	1:B:200:LEU:HD22	2.49	0.43
1:F:296:HIS:CD2	1:F:339:MET:HG3	2.54	0.43
1:L:405:VAL:O	1:L:406:LEU:HD23	2.19	0.43
1:C:224:GLY:N	1:C:225:PRO:CD	2.82	0.43
1:F:66:ALA:CB	1:F:187:THR:HG22	2.42	0.43
1:I:22:MET:HE1	1:I:31:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:LYS:CD	1:I:192:PRO:O	2.67	0.43
1:L:48:LEU:HD13	1:L:198:LEU:HD12	2.00	0.43
1:A:21:LYS:NZ	1:A:30:SER:OG	2.48	0.43
1:C:308:VAL:O	1:C:407:PRO:HA	2.19	0.43
1:G:22:MET:HE2	1:G:221:PRO:HD2	2.01	0.43
1:H:239:LYS:HE2	1:H:482:ASN:O	2.19	0.43
1:J:165:ILE:CG2	1:J:177:LYS:HG3	2.49	0.43
1:J:371:ARG:HD3	1:J:372:ALA:N	2.34	0.43
1:K:83:ARG:HD3	1:K:182:LEU:O	2.18	0.43
1:K:239:LYS:NZ	1:K:262:HIS:HD2	2.15	0.43
1:F:78:MET:HG2	1:F:82:GLU:CB	2.49	0.43
1:F:239:LYS:HZ3	1:F:262:HIS:HD2	1.66	0.43
1:L:84:ALA:HB2	1:L:135:THR:OG1	2.18	0.43
1:A:492:ASN:ND2	1:A:494:LYS:H	2.16	0.43
1:D:124:THR:HG22	1:D:172:VAL:HA	2.01	0.43
1:J:138:ILE:HG22	1:J:138:ILE:O	2.19	0.43
1:A:163:GLN:CD	1:A:177:LYS:HB3	2.44	0.43
1:E:253:MET:HE2	1:E:253:MET:HB2	1.81	0.43
1:F:48:LEU:HD11	1:F:107:LEU:HB3	2.01	0.43
1:H:433:ASN:HD22	1:H:436:THR:HG23	1.84	0.43
1:I:177:LYS:NZ	1:I:474:GLU:OE2	2.52	0.43
1:L:48:LEU:HD11	1:L:107:LEU:HB3	2.01	0.43
1:A:135:THR:HG22	1:A:183:ALA:HA	2.01	0.42
1:B:190:LEU:CD1	1:B:200:LEU:HD21	2.49	0.42
1:C:88:TYR:CD2	1:E:88:TYR:CE1	3.05	0.42
1:E:78:MET:CG	1:E:82:GLU:HB2	2.49	0.42
1:A:432:GLN:NE2	1:E:433:ASN:HD21	2.17	0.42
1:E:364:THR:HG21	1:E:386:ASP:OD2	2.19	0.42
1:F:451:ILE:O	1:F:452:ASN:HB2	2.19	0.42
1:A:471:ILE:HG13	1:C:260:ILE:HG22	2.00	0.42
1:B:253:MET:HE2	1:B:265:LEU:HD11	2.01	0.42
1:I:78:MET:CG	1:I:82:GLU:CB	2.97	0.42
1:I:296:HIS:O	1:I:401:PRO:HD3	2.18	0.42
1:D:169:PHE:O	1:D:173:MET:HG2	2.19	0.42
1:G:448:THR:HA	1:H:488:SER:O	2.20	0.42
1:I:364:THR:CG2	1:I:386:ASP:OD2	2.66	0.42
1:L:292:ILE:O	1:L:297:GLY:HA2	2.20	0.42
1:G:123:ALA:O	1:G:127:ASN:CG	2.63	0.42
1:G:124:THR:HG22	1:G:172:VAL:HB	2.01	0.42
1:G:163:GLN:OE1	1:G:188:ILE:HD13	2.20	0.42
1:G:387:VAL:CG1	1:G:388:THR:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:LYS:NZ	1:H:243:THR:CG2	2.83	0.42
1:J:78:MET:HG3	1:J:83:ARG:HG3	2.01	0.42
1:K:124:THR:HG21	1:K:171:LEU:HD13	2.01	0.42
1:A:239:LYS:NZ	1:A:264:THR:CG2	2.81	0.42
1:C:135:THR:OG1	1:C:136:THR:N	2.53	0.42
1:L:22:MET:HE3	1:L:24:ILE:HD12	2.00	0.42
1:L:199:SER:HB2	3:L:623:HOH:O	2.19	0.42
1:D:447:GLY:HA3	1:D:464:GLY:O	2.20	0.42
1:H:55:GLN:O	1:H:56:GLU:C	2.63	0.42
1:K:60:ASP:N	1:K:60:ASP:OD1	2.51	0.42
1:A:239:LYS:NZ	1:A:264:THR:HG23	2.35	0.42
1:B:107:LEU:HD13	1:B:333:MET:HG3	2.01	0.42
1:E:364:THR:HG23	1:E:386:ASP:OD2	2.19	0.42
1:J:123:ALA:O	1:J:127:ASN:CG	2.63	0.42
1:H:464:GLY:HA3	1:H:473:ARG:HD3	2.02	0.42
1:D:163:GLN:CB	1:D:190:LEU:HD23	2.50	0.42
1:G:348:GLN:HB2	1:G:377:TYR:HB3	2.01	0.42
1:K:387:VAL:HG13	1:K:394:VAL:HG11	2.02	0.42
1:K:447:GLY:HA3	1:K:464:GLY:O	2.20	0.42
1:L:433:ASN:HD22	1:L:436:THR:H	1.68	0.42
1:B:59:ILE:HD12	1:B:220:VAL:HG21	2.01	0.41
1:E:9:LYS:HE3	1:E:99:GLU:OE2	2.20	0.41
1:F:66:ALA:CB	1:F:187:THR:CG2	2.97	0.41
1:F:66:ALA:O	1:F:187:THR:HG21	2.20	0.41
1:F:167:TRP:CD2	1:F:343:VAL:HG11	2.54	0.41
1:G:281:LEU:HD12	1:G:281:LEU:HA	1.89	0.41
1:I:99:GLU:O	1:I:103:GLN:HG3	2.19	0.41
1:K:59:ILE:CD1	1:K:227:ALA:O	2.68	0.41
1:K:190:LEU:C	1:K:190:LEU:HD13	2.45	0.41
1:K:433:ASN:HD22	1:K:436:THR:HG23	1.85	0.41
1:L:364:THR:HG23	1:L:386:ASP:HB2	2.02	0.41
1:B:9:LYS:HB2	1:B:12:VAL:HG13	2.00	0.41
1:D:438:HIS:HD2	1:E:152:TYR:OH	2.03	0.41
1:G:191:LYS:HD3	1:G:192:PRO:O	2.21	0.41
1:G:311:LYS:HD2	1:G:312:HIS:NE2	2.34	0.41
1:L:167:TRP:CZ3	1:L:343:VAL:HB	2.54	0.41
1:C:235:HIS:HB3	3:C:775:HOH:O	2.21	0.41
1:F:299:ASN:HB3	1:F:302:ALA:HB2	2.01	0.41
1:J:177:LYS:NZ	1:J:474:GLU:OE2	2.45	0.41
1:K:17:ASN:C	1:K:18:GLU:OE2	2.63	0.41
1:J:17:ASN:OD1	1:J:17:ASN:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:354:TYR:OH	1:J:396:GLU:OE1	2.30	0.41
1:L:364:THR:HG23	1:L:386:ASP:OD2	2.20	0.41
1:A:88:TYR:CE1	1:D:88:TYR:CG	3.08	0.41
1:B:438:HIS:CE1	1:H:438:HIS:CE1	3.03	0.41
1:C:391:MET:HB2	1:C:394:VAL:HG13	2.02	0.41
1:J:8:LEU:HA	1:J:103:GLN:HE22	1.86	0.41
1:J:433:ASN:HB3	1:J:436:THR:CG2	2.48	0.41
1:A:324:ALA:O	1:A:327:VAL:HG13	2.20	0.41
1:D:92:ASP:O	1:D:96:GLU:HG3	2.21	0.41
1:F:188:ILE:CD1	1:F:190:LEU:CB	2.98	0.41
1:G:296:HIS:CD2	1:G:296:HIS:N	2.87	0.41
1:H:492:ASN:C	1:H:492:ASN:HD22	2.27	0.41
1:J:372:ALA:HB2	1:J:380:LYS:HG3	2.03	0.41
1:J:404:VAL:CG1	1:J:406:LEU:HD11	2.51	0.41
1:K:190:LEU:HD12	1:K:200:LEU:HD21	2.03	0.41
1:B:277:GLU:O	1:B:312:HIS:HE1	2.03	0.41
1:B:342:LEU:HB2	1:B:377:TYR:O	2.21	0.41
1:D:152:TYR:OH	1:E:438:HIS:HD2	2.03	0.41
1:G:22:MET:HE2	1:G:22:MET:HB3	1.86	0.41
1:A:88:TYR:CE1	1:D:88:TYR:CD2	3.08	0.41
1:B:254:ARG:HG3	1:I:254:ARG:HG3	2.01	0.41
1:B:260:ILE:HD12	1:B:260:ILE:N	2.35	0.41
1:D:107:LEU:HD13	1:D:333:MET:CG	2.46	0.41
1:F:235:HIS:CA	1:F:259:MET:HE3	2.38	0.41
1:G:177:LYS:HZ1	1:G:243:THR:HG22	1.85	0.41
1:J:308:VAL:HG21	1:J:316:VAL:CG2	2.46	0.41
1:H:112:PRO:HB2	1:H:115:VAL:HG13	2.02	0.41
1:H:329:LEU:HD12	1:H:339:MET:HB3	2.02	0.41
1:I:124:THR:HG22	1:I:172:VAL:HA	2.02	0.41
1:I:357:GLN:O	1:I:357:GLN:HG3	2.21	0.41
1:J:434:ILE:HA	1:K:434:ILE:HB	2.01	0.41
1:B:492:ASN:ND2	1:B:494:LYS:H	2.19	0.41
1:E:78:MET:HE3	1:E:78:MET:HB2	1.90	0.41
1:F:308:VAL:HG11	1:F:316:VAL:HG13	2.02	0.41
1:H:239:LYS:NZ	1:H:262:HIS:CD2	2.87	0.41
1:B:88:TYR:CZ	1:G:88:TYR:CD2	3.09	0.40
1:D:107:LEU:CD1	1:D:333:MET:HG3	2.47	0.40
1:E:259:MET:HE3	1:E:261:LYS:HE3	2.03	0.40
1:F:59:ILE:N	1:F:59:ILE:HD13	2.36	0.40
1:L:135:THR:OG1	1:L:136:THR:N	2.54	0.40
1:H:264:THR:CG2	1:H:264:THR:OG1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:ILE:HG12	1:I:284:ALA:HB1	2.03	0.40
1:L:161:VAL:HG21	1:L:483:TYR:HE1	1.86	0.40
1:E:357:GLN:HE22	1:E:360:LYS:NZ	2.18	0.40
1:F:277:GLU:O	1:F:312:HIS:HE1	2.04	0.40
1:G:177:LYS:HZ1	1:G:243:THR:CG2	2.34	0.40
1:G:492:ASN:ND2	1:G:494:LYS:H	2.19	0.40
1:I:371:ARG:NH1	1:I:372:ALA:O	2.50	0.40
1:J:433:ASN:HD22	1:J:436:THR:H	1.68	0.40
1:K:134:TRP:CG	1:K:480:LEU:HD11	2.56	0.40
1:K:296:HIS:CD2	1:K:296:HIS:N	2.89	0.40
1:L:407:PRO:O	1:L:417:ARG:NH1	2.47	0.40
1:L:426:ALA:HA	1:L:448:THR:O	2.22	0.40
1:A:107:LEU:HD13	1:A:333:MET:HG3	2.03	0.40
1:F:177:LYS:NZ	1:F:243:THR:CG2	2.84	0.40
1:G:438:HIS:CE1	1:I:438:HIS:CE1	3.06	0.40
1:I:345:LYS:HE3	1:I:349:GLU:OE2	2.22	0.40
1:I:492:ASN:ND2	1:I:494:LYS:H	2.19	0.40
1:B:484:THR:HG22	3:B:634:HOH:O	2.21	0.40
1:C:492:ASN:C	1:C:492:ASN:ND2	2.80	0.40
1:D:260:ILE:HD12	1:E:468:GLN:HB3	2.03	0.40
1:E:124:THR:HG22	1:E:172:VAL:HA	2.02	0.40
1:I:492:ASN:C	1:I:492:ASN:HD22	2.30	0.40
1:J:364:THR:O	1:J:384:PHE:HA	2.22	0.40
1:K:17:ASN:O	1:K:18:GLU:OE2	2.40	0.40
1:K:484:THR:HG22	1:K:485:GLU:N	2.37	0.40
1:L:67:ARG:O	1:L:71:GLU:HG2	2.21	0.40
1:L:124:THR:HG21	1:L:171:LEU:HD13	2.04	0.40
1:L:321:VAL:HG13	1:L:367:ALA:HB2	2.03	0.40
1:L:342:LEU:HD12	1:L:342:LEU:HA	1.85	0.40
1:L:492:ASN:C	1:L:492:ASN:ND2	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/494 (99%)	478 (98%)	12 (2%)	0	100	100
1	B	490/494 (99%)	471 (96%)	19 (4%)	0	100	100
1	C	490/494 (99%)	476 (97%)	13 (3%)	1 (0%)	43	36
1	D	490/494 (99%)	476 (97%)	14 (3%)	0	100	100
1	E	488/494 (99%)	474 (97%)	14 (3%)	0	100	100
1	F	491/494 (99%)	475 (97%)	16 (3%)	0	100	100
1	G	488/494 (99%)	473 (97%)	15 (3%)	0	100	100
1	H	489/494 (99%)	473 (97%)	16 (3%)	0	100	100
1	I	489/494 (99%)	471 (96%)	18 (4%)	0	100	100
1	J	489/494 (99%)	471 (96%)	17 (4%)	1 (0%)	43	36
1	K	487/494 (99%)	470 (96%)	17 (4%)	0	100	100
1	L	486/494 (98%)	466 (96%)	18 (4%)	2 (0%)	30	22
All	All	5867/5928 (99%)	5674 (97%)	189 (3%)	4 (0%)	48	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	78	MET
1	C	373	LEU
1	L	424	GLY
1	J	424	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/401 (100%)	373 (94%)	26 (6%)	15	8
1	B	399/401 (100%)	367 (92%)	32 (8%)	11	5
1	C	399/401 (100%)	370 (93%)	29 (7%)	13	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	399/401 (100%)	370 (93%)	29 (7%)	13	6
1	E	397/401 (99%)	371 (94%)	26 (6%)	15	8
1	F	400/401 (100%)	367 (92%)	33 (8%)	10	4
1	G	397/401 (99%)	364 (92%)	33 (8%)	10	4
1	H	398/401 (99%)	355 (89%)	43 (11%)	6	2
1	I	398/401 (99%)	367 (92%)	31 (8%)	11	5
1	J	398/401 (99%)	354 (89%)	44 (11%)	6	2
1	K	396/401 (99%)	352 (89%)	44 (11%)	6	2
1	L	395/401 (98%)	347 (88%)	48 (12%)	5	2
All	All	4775/4812 (99%)	4357 (91%)	418 (9%)	9	4

All (418) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	18	GLU
1	A	59	ILE
1	A	71	GLU
1	A	104	LEU
1	A	105	GLU
1	A	107	LEU
1	A	115	VAL
1	A	121	ILE
1	A	124	THR
1	A	158	VAL
1	A	166	PRO
1	A	171	LEU
1	A	264	THR
1	A	296	HIS
1	A	316	VAL
1	A	327	VAL
1	A	329	LEU
1	A	336	GLU
1	A	342	LEU
1	A	375	LYS
1	A	387	VAL
1	A	394	VAL
1	A	484	THR
1	A	492	ASN

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Mol	Chain	Res	Type
1	A	493	ILE
1	B	12	VAL
1	B	18	GLU
1	B	20	ILE
1	B	48	LEU
1	B	71	GLU
1	B	104	LEU
1	B	105	GLU
1	B	107	LEU
1	B	115	VAL
1	B	121	ILE
1	B	124	THR
1	B	147	LYS
1	B	158	VAL
1	B	166	PRO
1	B	171	LEU
1	B	190	LEU
1	B	217	VAL
1	B	290	GLN
1	B	296	HIS
1	B	306	VAL
1	B	311	LYS
1	B	316	VAL
1	B	327	VAL
1	B	335	LYS
1	B	342	LEU
1	B	379	VAL
1	B	387	VAL
1	B	390	ASP
1	B	394	VAL
1	B	448	THR
1	B	484	THR
1	B	492	ASN
1	C	4	THR
1	C	8	LEU
1	C	27	GLU
1	C	48	LEU
1	C	71	GLU
1	C	77	GLU
1	C	107	LEU
1	C	121	ILE
1	C	158	VAL

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Mol	Chain	Res	Type
1	C	171	LEU
1	C	187	THR
1	C	247	VAL
1	C	258	GLU
1	C	296	HIS
1	C	311	LYS
1	C	316	VAL
1	C	335	LYS
1	C	353	ASN
1	C	359	LYS
1	C	360	LYS
1	C	364	THR
1	C	365	VAL
1	C	371	ARG
1	C	374	GLU
1	C	375	LYS
1	C	379	VAL
1	C	394	VAL
1	C	492	ASN
1	C	494	LYS
1	D	7	GLU
1	D	8	LEU
1	D	71	GLU
1	D	105	GLU
1	D	107	LEU
1	D	109	ASN
1	D	121	ILE
1	D	124	THR
1	D	147	LYS
1	D	158	VAL
1	D	161	VAL
1	D	171	LEU
1	D	217	VAL
1	D	282	GLU
1	D	290	GLN
1	D	296	HIS
1	D	311	LYS
1	D	316	VAL
1	D	321	VAL
1	D	350	ARG
1	D	364	THR
1	D	365	VAL

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Mol	Chain	Res	Type
1	D	371	ARG
1	D	375	LYS
1	D	385	THR
1	D	387	VAL
1	D	394	VAL
1	D	484	THR
1	D	492	ASN
1	E	7	GLU
1	E	13	GLU
1	E	71	GLU
1	E	104	LEU
1	E	105	GLU
1	E	107	LEU
1	E	109	ASN
1	E	124	THR
1	E	171	LEU
1	E	172	VAL
1	E	187	THR
1	E	188	ILE
1	E	190	LEU
1	E	194	SER
1	E	217	VAL
1	E	253	MET
1	E	296	HIS
1	E	310	ARG
1	E	327	VAL
1	E	329	LEU
1	E	364	THR
1	E	371	ARG
1	E	375	LYS
1	E	394	VAL
1	E	412	GLU
1	E	492	ASN
1	F	13	GLU
1	F	17	ASN
1	F	18	GLU
1	F	35	LYS
1	F	48	LEU
1	F	59	ILE
1	F	71	GLU
1	F	77	GLU
1	F	104	LEU

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Mol	Chain	Res	Type
1	F	105	GLU
1	F	107	LEU
1	F	115	VAL
1	F	171	LEU
1	F	187	THR
1	F	188	ILE
1	F	217	VAL
1	F	225	PRO
1	F	243	THR
1	F	246	THR
1	F	296	HIS
1	F	301	SER
1	F	316	VAL
1	F	327	VAL
1	F	329	LEU
1	F	351	VAL
1	F	371	ARG
1	F	375	LYS
1	F	399	PHE
1	F	412	GLU
1	F	457	GLU
1	F	484	THR
1	F	492	ASN
1	F	494	LYS
1	G	7	GLU
1	G	8	LEU
1	G	9	LYS
1	G	27	GLU
1	G	71	GLU
1	G	105	GLU
1	G	107	LEU
1	G	109	ASN
1	G	115	VAL
1	G	124	THR
1	G	158	VAL
1	G	171	LEU
1	G	172	VAL
1	G	188	ILE
1	G	194	SER
1	G	205	LYS
1	G	217	VAL
1	G	243	THR

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Mol	Chain	Res	Type
1	G	246	THR
1	G	264	THR
1	G	290	GLN
1	G	296	HIS
1	G	311	LYS
1	G	316	VAL
1	G	327	VAL
1	G	329	LEU
1	G	342	LEU
1	G	360	LYS
1	G	364	THR
1	G	375	LYS
1	G	394	VAL
1	G	406	LEU
1	G	492	ASN
1	H	8	LEU
1	H	13	GLU
1	H	27	GLU
1	H	35	LYS
1	H	48	LEU
1	H	71	GLU
1	H	83	ARG
1	H	104	LEU
1	H	105	GLU
1	H	107	LEU
1	H	115	VAL
1	H	121	ILE
1	H	124	THR
1	H	158	VAL
1	H	171	LEU
1	H	172	VAL
1	H	187	THR
1	H	188	ILE
1	H	217	VAL
1	H	243	THR
1	H	246	THR
1	H	247	VAL
1	H	248	THR
1	H	264	THR
1	H	282	GLU
1	H	296	HIS
1	H	316	VAL

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Mol	Chain	Res	Type
1	H	327	VAL
1	H	329	LEU
1	H	342	LEU
1	H	351	VAL
1	H	353	ASN
1	H	364	THR
1	H	365	VAL
1	H	371	ARG
1	H	375	LYS
1	H	385	THR
1	H	394	VAL
1	H	412	GLU
1	H	429	VAL
1	H	445	LYS
1	H	484	THR
1	H	492	ASN
1	I	4	THR
1	I	8	LEU
1	I	18	GLU
1	I	27	GLU
1	I	48	LEU
1	I	50	VAL
1	I	60	ASP
1	I	104	LEU
1	I	107	LEU
1	I	115	VAL
1	I	121	ILE
1	I	124	THR
1	I	147	LYS
1	I	171	LEU
1	I	191	LYS
1	I	246	THR
1	I	252	ILE
1	I	266	GLU
1	I	292	ILE
1	I	296	HIS
1	I	301	SER
1	I	311	LYS
1	I	316	VAL
1	I	322	LYS
1	I	342	LEU
1	I	346	LYS

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Mol	Chain	Res	Type
1	I	364	THR
1	I	371	ARG
1	I	375	LYS
1	I	484	THR
1	I	492	ASN
1	J	9	LYS
1	J	12	VAL
1	J	13	GLU
1	J	18	GLU
1	J	19	GLU
1	J	27	GLU
1	J	48	LEU
1	J	59	ILE
1	J	71	GLU
1	J	104	LEU
1	J	105	GLU
1	J	107	LEU
1	J	115	VAL
1	J	121	ILE
1	J	171	LEU
1	J	172	VAL
1	J	173	MET
1	J	188	ILE
1	J	245	SER
1	J	247	VAL
1	J	259	MET
1	J	296	HIS
1	J	301	SER
1	J	316	VAL
1	J	327	VAL
1	J	328	LYS
1	J	329	LEU
1	J	342	LEU
1	J	351	VAL
1	J	353	ASN
1	J	359	LYS
1	J	360	LYS
1	J	364	THR
1	J	365	VAL
1	J	371	ARG
1	J	387	VAL
1	J	404	VAL

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Mol	Chain	Res	Type
1	J	405	VAL
1	J	412	GLU
1	J	435	LYS
1	J	436	THR
1	J	448	THR
1	J	484	THR
1	J	492	ASN
1	K	8	LEU
1	K	12	VAL
1	K	18	GLU
1	K	21	LYS
1	K	27	GLU
1	K	48	LEU
1	K	60	ASP
1	K	71	GLU
1	K	77	GLU
1	K	104	LEU
1	K	107	LEU
1	K	115	VAL
1	K	124	THR
1	K	158	VAL
1	K	161	VAL
1	K	171	LEU
1	K	172	VAL
1	K	187	THR
1	K	188	ILE
1	K	190	LEU
1	K	194	SER
1	K	217	VAL
1	K	220	VAL
1	K	232	VAL
1	K	246	THR
1	K	252	ILE
1	K	316	VAL
1	K	327	VAL
1	K	328	LYS
1	K	329	LEU
1	K	335	LYS
1	K	342	LEU
1	K	343	VAL
1	K	353	ASN
1	K	359	LYS

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Mol	Chain	Res	Type
1	K	360	LYS
1	K	364	THR
1	K	375	LYS
1	K	380	LYS
1	K	387	VAL
1	K	394	VAL
1	K	429	VAL
1	K	435	LYS
1	K	492	ASN
1	L	7	GLU
1	L	8	LEU
1	L	9	LYS
1	L	13	GLU
1	L	22	MET
1	L	32	ILE
1	L	48	LEU
1	L	50	VAL
1	L	104	LEU
1	L	105	GLU
1	L	107	LEU
1	L	115	VAL
1	L	124	THR
1	L	126	GLU
1	L	158	VAL
1	L	171	LEU
1	L	187	THR
1	L	190	LEU
1	L	191	LYS
1	L	217	VAL
1	L	218	ASN
1	L	232	VAL
1	L	239	LYS
1	L	243	THR
1	L	246	THR
1	L	248	THR
1	L	290	GLN
1	L	296	HIS
1	L	316	VAL
1	L	342	LEU
1	L	345	LYS
1	L	353	ASN
1	L	364	THR

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Mol	Chain	Res	Type
1	L	375	LYS
1	L	381	PRO
1	L	385	THR
1	L	405	VAL
1	L	412	GLU
1	L	422	SER
1	L	429	VAL
1	L	431	THR
1	L	434	ILE
1	L	436	THR
1	L	445	LYS
1	L	448	THR
1	L	471	ILE
1	L	484	THR
1	L	492	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	103	GLN
1	A	114	GLN
1	A	141	GLN
1	A	214	ASN
1	A	233	ASN
1	A	255	GLN
1	A	262	HIS
1	A	312	HIS
1	A	326	ASN
1	A	347	GLN
1	A	353	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN
1	A	482	ASN
1	A	492	ASN
1	B	85	HIS
1	B	103	GLN
1	B	114	GLN
1	B	141	GLN
1	B	151	ASN

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Mol	Chain	Res	Type
1	B	214	ASN
1	B	233	ASN
1	B	255	GLN
1	B	262	HIS
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	357	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	442	ASN
1	B	482	ASN
1	B	492	ASN
1	C	55	GLN
1	C	85	HIS
1	C	103	GLN
1	C	114	GLN
1	C	141	GLN
1	C	214	ASN
1	C	233	ASN
1	C	255	GLN
1	C	262	HIS
1	C	312	HIS
1	C	326	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	482	ASN
1	C	492	ASN
1	D	103	GLN
1	D	114	GLN
1	D	141	GLN
1	D	214	ASN
1	D	255	GLN
1	D	262	HIS
1	D	299	ASN
1	D	326	ASN
1	D	347	GLN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS

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Mol	Chain	Res	Type
1	D	482	ASN
1	D	492	ASN
1	E	103	GLN
1	E	114	GLN
1	E	214	ASN
1	E	255	GLN
1	E	262	HIS
1	E	312	HIS
1	E	325	ASN
1	E	326	ASN
1	E	348	GLN
1	E	357	GLN
1	E	432	GLN
1	E	438	HIS
1	E	442	ASN
1	E	482	ASN
1	E	492	ASN
1	F	103	GLN
1	F	114	GLN
1	F	262	HIS
1	F	298	GLN
1	F	312	HIS
1	F	325	ASN
1	F	353	ASN
1	F	357	GLN
1	F	432	GLN
1	F	433	ASN
1	F	438	HIS
1	F	482	ASN
1	F	492	ASN
1	G	85	HIS
1	G	103	GLN
1	G	114	GLN
1	G	141	GLN
1	G	214	ASN
1	G	233	ASN
1	G	255	GLN
1	G	262	HIS
1	G	312	HIS
1	G	326	ASN
1	G	353	ASN
1	G	357	GLN

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Mol	Chain	Res	Type
1	G	432	GLN
1	G	433	ASN
1	G	438	HIS
1	G	482	ASN
1	G	492	ASN
1	H	85	HIS
1	H	103	GLN
1	H	114	GLN
1	H	141	GLN
1	H	214	ASN
1	H	235	HIS
1	H	262	HIS
1	H	312	HIS
1	H	325	ASN
1	H	326	ASN
1	H	357	GLN
1	H	432	GLN
1	H	433	ASN
1	H	438	HIS
1	H	482	ASN
1	H	492	ASN
1	I	85	HIS
1	I	103	GLN
1	I	141	GLN
1	I	214	ASN
1	I	262	HIS
1	I	299	ASN
1	I	312	HIS
1	I	326	ASN
1	I	432	GLN
1	I	433	ASN
1	I	438	HIS
1	I	442	ASN
1	I	482	ASN
1	I	492	ASN
1	J	85	HIS
1	J	103	GLN
1	J	114	GLN
1	J	141	GLN
1	J	214	ASN
1	J	262	HIS
1	J	286	ASN

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Mol	Chain	Res	Type
1	J	290	GLN
1	J	312	HIS
1	J	325	ASN
1	J	326	ASN
1	J	347	GLN
1	J	432	GLN
1	J	433	ASN
1	J	438	HIS
1	J	492	ASN
1	K	103	GLN
1	K	141	GLN
1	K	214	ASN
1	K	233	ASN
1	K	255	GLN
1	K	262	HIS
1	K	286	ASN
1	K	290	GLN
1	K	298	GLN
1	K	325	ASN
1	K	326	ASN
1	K	433	ASN
1	K	438	HIS
1	K	442	ASN
1	K	492	ASN
1	L	103	GLN
1	L	114	GLN
1	L	151	ASN
1	L	214	ASN
1	L	262	HIS
1	L	298	GLN
1	L	312	HIS
1	L	326	ASN
1	L	347	GLN
1	L	432	GLN
1	L	433	ASN
1	L	438	HIS
1	L	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	491/494 (99%)	-0.17	6 (1%) 76 79	5, 10, 21, 35	1 (0%)
1	B	491/494 (99%)	0.37	12 (2%) 59 63	10, 17, 30, 45	1 (0%)
1	C	491/494 (99%)	-0.06	4 (0%) 82 85	5, 12, 25, 43	1 (0%)
1	D	489/494 (98%)	-0.07	6 (1%) 76 79	3, 12, 25, 37	3 (0%)
1	E	490/494 (99%)	-0.13	8 (1%) 70 74	5, 11, 23, 43	0
1	F	491/494 (99%)	0.47	11 (2%) 62 66	9, 17, 31, 43	2 (0%)
1	G	490/494 (99%)	0.30	16 (3%) 49 52	10, 16, 29, 52	0
1	H	490/494 (99%)	0.30	10 (2%) 65 69	10, 16, 29, 58	1 (0%)
1	I	491/494 (99%)	0.41	9 (1%) 67 71	11, 18, 30, 46	0
1	J	491/494 (99%)	0.65	20 (4%) 41 44	10, 21, 34, 53	0
1	K	489/494 (98%)	0.85	31 (6%) 26 27	13, 21, 34, 50	0
1	L	488/494 (98%)	0.97	45 (9%) 14 15	13, 22, 35, 57	0
All	All	5882/5928 (99%)	0.32	178 (3%) 52 56	3, 17, 30, 58	9 (0%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	247	VAL	6.4
1	K	247	VAL	5.4
1	C	4	THR	5.2
1	G	247	VAL	5.0
1	J	4	THR	5.0
1	C	88	TYR	4.7
1	A	247	VAL	4.6
1	L	43	ALA	4.6
1	I	247	VAL	4.6
1	J	247	VAL	4.1
1	E	5	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	390	ASP	4.0
1	L	235	HIS	4.0
1	F	88	TYR	3.9
1	L	351	VAL	3.9
1	E	88	TYR	3.8
1	I	88	TYR	3.7
1	D	7	GLU	3.6
1	I	259	MET	3.6
1	I	4	THR	3.6
1	J	8	LEU	3.6
1	H	246	THR	3.5
1	L	66	ALA	3.5
1	L	88	TYR	3.5
1	D	247	VAL	3.5
1	L	7	GLU	3.5
1	J	33	GLY	3.5
1	L	246	THR	3.5
1	E	247	VAL	3.5
1	G	5	ASN	3.4
1	H	5	ASN	3.4
1	G	246	THR	3.4
1	L	247	VAL	3.3
1	A	88	TYR	3.3
1	L	29	VAL	3.3
1	D	88	TYR	3.2
1	K	246	THR	3.1
1	B	88	TYR	3.1
1	C	374	GLU	3.1
1	J	390	ASP	3.0
1	K	6	ILE	3.0
1	B	235	HIS	2.9
1	B	247	VAL	2.9
1	H	247	VAL	2.9
1	K	282	GLU	2.9
1	G	6	ILE	2.9
1	J	32	ILE	2.9
1	G	88	TYR	2.9
1	F	246	THR	2.9
1	H	259	MET	2.9
1	A	259	MET	2.9
1	C	247	VAL	2.9
1	L	158	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	246	THR	2.9
1	F	69	ALA	2.9
1	G	7	GLU	2.8
1	K	336	GLU	2.8
1	K	194	SER	2.8
1	F	4	THR	2.8
1	K	373	LEU	2.8
1	L	194	SER	2.8
1	K	115	VAL	2.8
1	L	387	VAL	2.7
1	G	35	LYS	2.7
1	H	257	ALA	2.7
1	L	40	TYR	2.7
1	F	235	HIS	2.7
1	J	362	GLY	2.7
1	B	4	THR	2.7
1	K	318	ASP	2.7
1	F	494	LYS	2.7
1	L	335	LYS	2.7
1	H	88	TYR	2.7
1	A	126	GLU	2.7
1	H	6	ILE	2.7
1	K	281	LEU	2.6
1	J	335	LYS	2.6
1	L	50	VAL	2.6
1	K	335	LYS	2.6
1	K	248	THR	2.6
1	G	235	HIS	2.5
1	L	423	TYR	2.5
1	L	37	PHE	2.5
1	L	70	PHE	2.5
1	J	373	LEU	2.5
1	A	4	THR	2.5
1	J	248	THR	2.5
1	L	254	ARG	2.5
1	B	259	MET	2.5
1	L	264	THR	2.5
1	G	335	LYS	2.5
1	K	88	TYR	2.4
1	G	412	GLU	2.4
1	K	260	ILE	2.4
1	I	363	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	365	VAL	2.4
1	K	297	GLY	2.4
1	L	494	LYS	2.4
1	L	35	LYS	2.4
1	B	390	ASP	2.4
1	F	412	GLU	2.4
1	B	357	GLN	2.4
1	K	222	GLY	2.4
1	L	26	GLY	2.4
1	G	147	LYS	2.4
1	J	406	LEU	2.3
1	J	364	THR	2.3
1	H	350	ARG	2.3
1	G	8	LEU	2.3
1	L	281	LEU	2.3
1	J	246	THR	2.3
1	K	363	ALA	2.3
1	B	32	ILE	2.3
1	K	32	ILE	2.3
1	E	290	GLN	2.3
1	L	290	GLN	2.3
1	D	494	LYS	2.3
1	F	54	ALA	2.3
1	L	446	ALA	2.3
1	F	32	ILE	2.3
1	J	176	TRP	2.2
1	K	423	TYR	2.2
1	L	381	PRO	2.2
1	L	470	GLY	2.2
1	F	245	SER	2.2
1	I	248	THR	2.2
1	L	135	THR	2.2
1	J	14	ALA	2.2
1	J	463	PHE	2.2
1	K	251	TYR	2.2
1	B	471	ILE	2.2
1	G	371	ARG	2.2
1	E	314	GLU	2.2
1	D	246	THR	2.2
1	K	44	THR	2.2
1	L	59	ILE	2.2
1	L	164	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	35	LYS	2.2
1	L	360	LYS	2.2
1	E	282	GLU	2.2
1	B	387	VAL	2.2
1	I	158	VAL	2.2
1	J	414	VAL	2.2
1	L	47	VAL	2.2
1	K	346	LYS	2.2
1	E	412	GLU	2.1
1	G	290	GLN	2.1
1	K	436	THR	2.1
1	L	383	VAL	2.1
1	B	8	LEU	2.1
1	L	350	ARG	2.1
1	A	235	HIS	2.1
1	I	283	GLU	2.1
1	J	433	ASN	2.1
1	L	32	ILE	2.1
1	H	264	THR	2.1
1	K	134	TRP	2.1
1	J	115	VAL	2.1
1	L	343	VAL	2.1
1	L	358	GLY	2.1
1	I	35	LYS	2.1
1	G	314	GLU	2.1
1	L	333	MET	2.1
1	L	401	PRO	2.1
1	K	61	ALA	2.1
1	G	194	SER	2.1
1	K	12	VAL	2.1
1	K	217	VAL	2.1
1	L	8	LEU	2.1
1	D	6	ILE	2.0
1	L	251	TYR	2.0
1	K	224	GLY	2.0
1	H	17	ASN	2.0
1	K	117	LEU	2.0
1	L	86	LEU	2.0
1	L	377	TYR	2.0
1	J	402	VAL	2.0
1	K	321	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	B	501	1/1	0.86	0.12	17,17,17,17	0
2	NA	F	501	1/1	0.90	0.07	16,16,16,16	0
2	NA	K	501	1/1	0.92	0.15	20,20,20,20	0
2	NA	K	502	1/1	0.92	0.16	23,23,23,23	0
2	NA	J	502	1/1	0.93	0.11	21,21,21,21	0
2	NA	L	501	1/1	0.93	0.15	21,21,21,21	0
2	NA	J	501	1/1	0.94	0.20	20,20,20,20	0
2	NA	I	501	1/1	0.95	0.08	19,19,19,19	0
2	NA	B	502	1/1	0.95	0.06	14,14,14,14	0
2	NA	I	502	1/1	0.96	0.10	15,15,15,15	0
2	NA	C	501	1/1	0.96	0.05	12,12,12,12	0
2	NA	D	501	1/1	0.97	0.05	11,11,11,11	0
2	NA	A	501	1/1	0.97	0.10	10,10,10,10	0
2	NA	F	502	1/1	0.97	0.05	13,13,13,13	0
2	NA	G	501	1/1	0.97	0.03	14,14,14,14	0
2	NA	H	501	1/1	0.97	0.07	15,15,15,15	0
2	NA	C	502	1/1	0.97	0.06	9,9,9,9	0
2	NA	L	502	1/1	0.97	0.06	23,23,23,23	0
2	NA	H	502	1/1	0.98	0.06	16,16,16,16	0
2	NA	D	502	1/1	0.98	0.06	12,12,12,12	0
2	NA	E	501	1/1	0.98	0.09	10,10,10,10	0
2	NA	A	502	1/1	0.99	0.02	10,10,10,10	0
2	NA	G	502	1/1	0.99	0.04	15,15,15,15	0
2	NA	E	502	1/1	0.99	0.05	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.