



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:01 AM UTC

PDB ID : 3BFJ / pdb_00003bfj
Title : Crystal structure analysis of 1,3-propanediol oxidoreductase
Authors : Marcal, D.; Enguita, F.J.; Carrondo, M.A.; Structural Proteomics in Europe (SPINE)
Deposited on : 2007-11-21
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

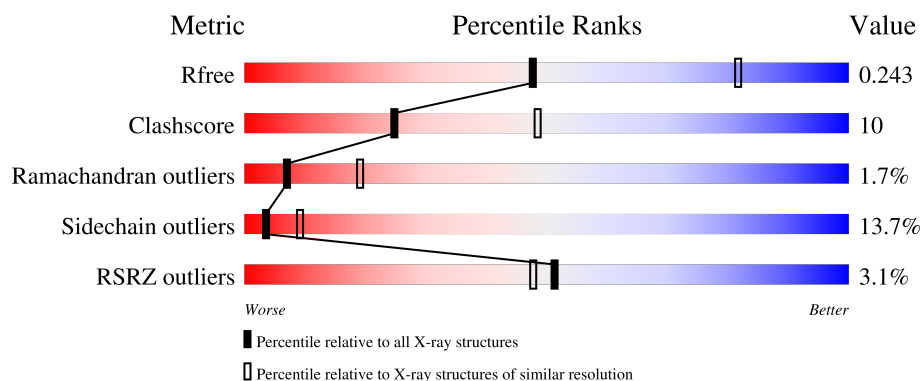
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	387	3% 73% 22% ...
1	B	387	2% 72% 21% 5% .
1	C	387	2% 75% 21% ...
1	D	387	2% 73% 20% 6% .
1	E	387	3% 74% 20% 5% .

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Mol	Chain	Length	Quality of chain
1	F	387	
1	G	387	
1	H	387	
1	I	387	
1	J	387	
1	K	387	
1	L	387	
1	M	387	
1	N	387	
1	O	387	
1	P	387	
1	Q	387	
1	R	387	
1	S	387	
1	T	387	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 58348 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 1,3-propanediol oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	B	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	C	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	D	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	E	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	F	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	G	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	H	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	I	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	J	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	K	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	L	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	M	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	N	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	O	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	P	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	R	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	S	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			
1	T	382	Total	C	N	O	S	0	0	0
			2871	1810	505	540	16			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		
2	G	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		
2	M	1	Total	Fe	0	0
			1	1		
2	N	1	Total	Fe	0	0
			1	1		
2	O	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total 1	Fe 1	0	0
2	Q	1	Total 1	Fe 1	0	0
2	R	1	Total 1	Fe 1	0	0
2	S	1	Total 1	Fe 1	0	0
2	T	1	Total 1	Fe 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total 36	O 36	0	0
3	B	45	Total 45	O 45	0	0
3	C	27	Total 27	O 27	0	0
3	D	49	Total 49	O 49	0	0
3	E	76	Total 76	O 76	0	0
3	F	19	Total 19	O 19	0	0
3	G	41	Total 41	O 41	0	0
3	H	61	Total 61	O 61	0	0
3	I	51	Total 51	O 51	0	0
3	J	31	Total 31	O 31	0	0
3	K	89	Total 89	O 89	0	0
3	L	42	Total 42	O 42	0	0
3	M	58	Total 58	O 58	0	0
3	N	33	Total 33	O 33	0	0

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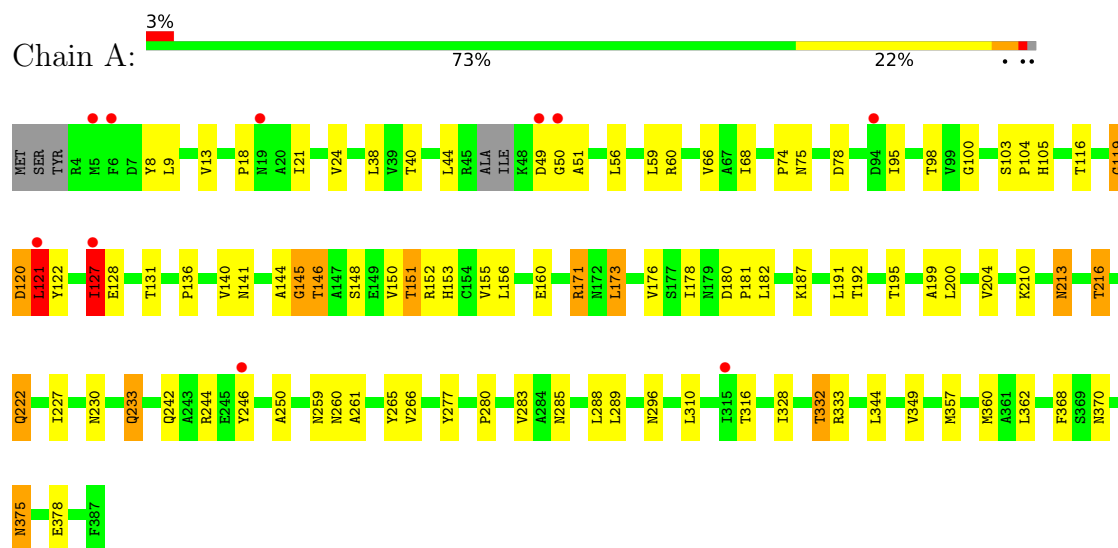
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	50	Total 50	O 50	0	0
3	P	64	Total 64	O 64	0	0
3	Q	43	Total 43	O 43	0	0
3	R	39	Total 39	O 39	0	0
3	S	19	Total 19	O 19	0	0
3	T	35	Total 35	O 35	0	0

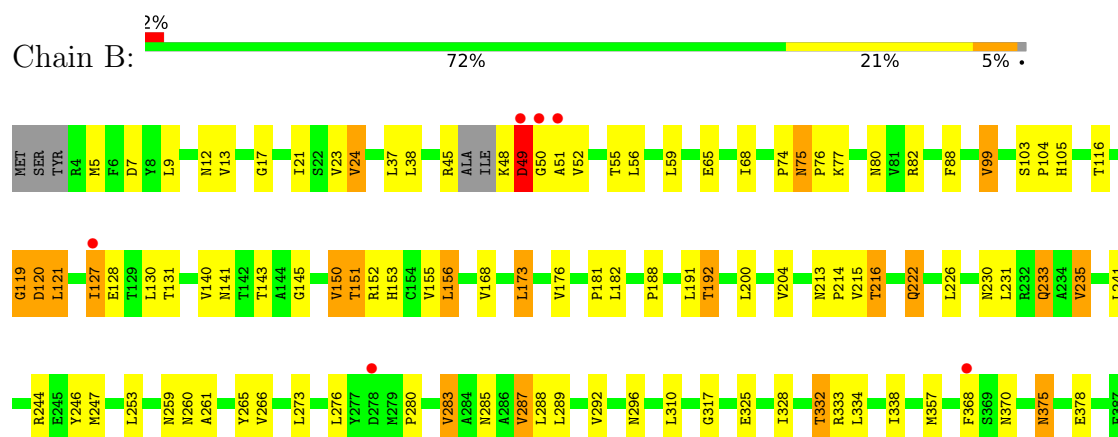
3 Residue-property plots [i](#)

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.

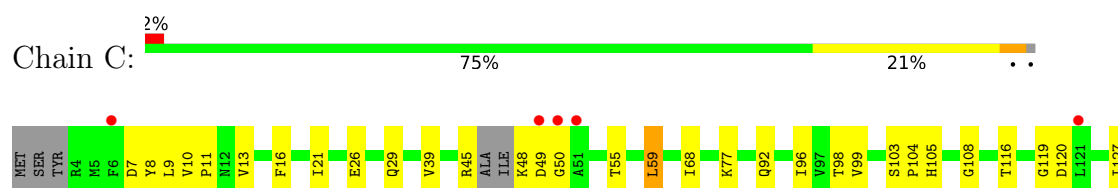
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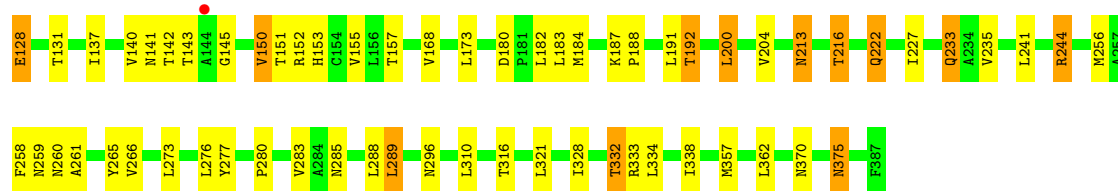


- Molecule 1: 1,3-propanediol oxidoreductase

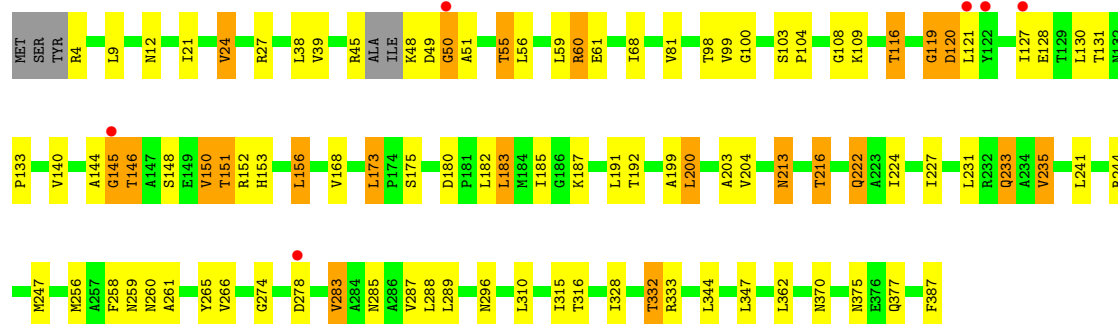


- Molecule 1: 1,3-propanediol oxidoreductase

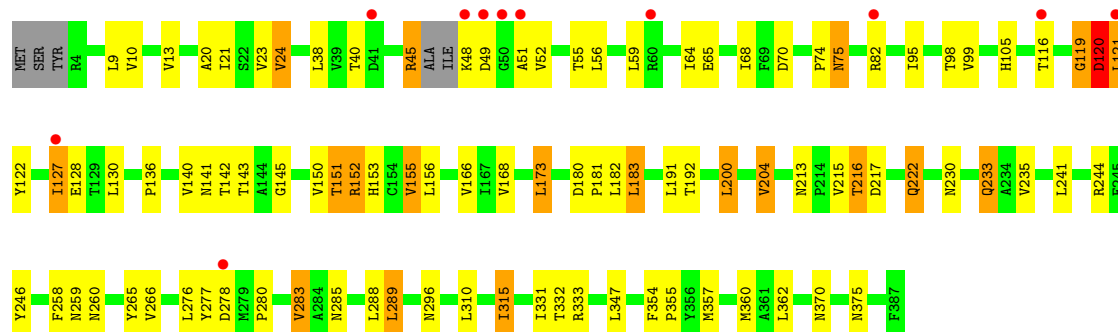
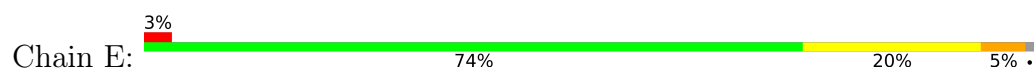




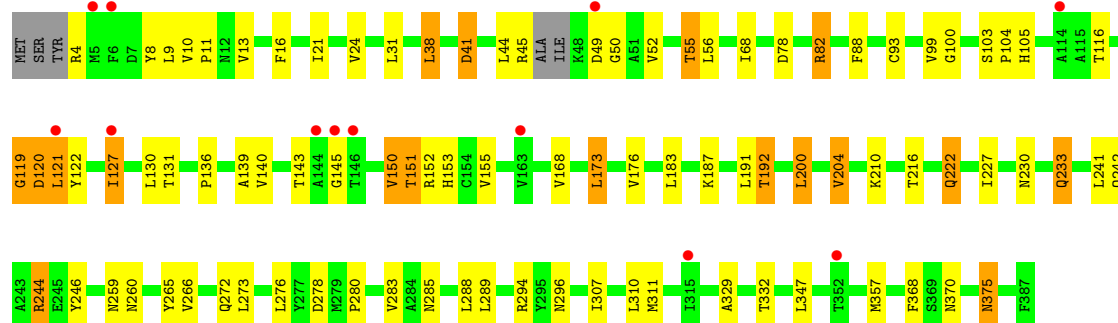
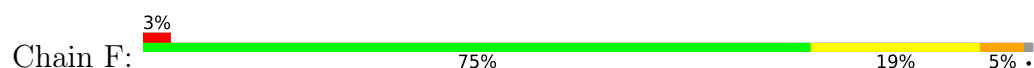
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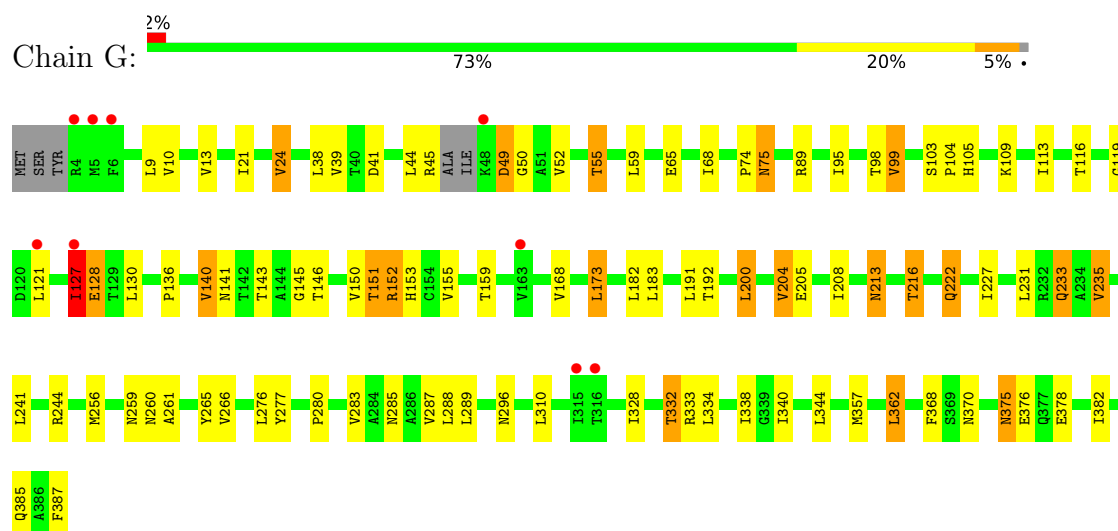
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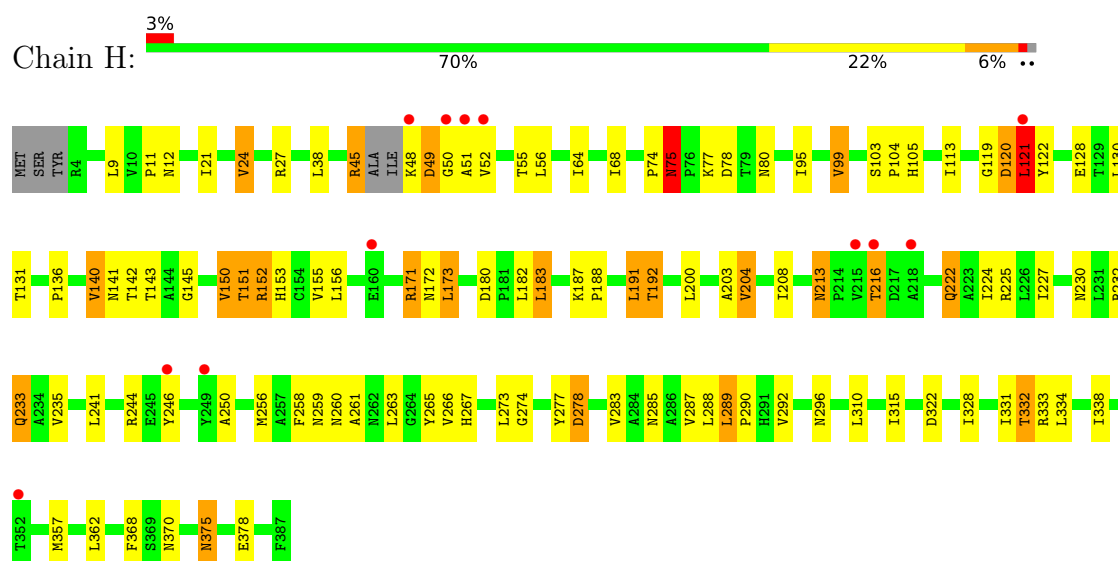
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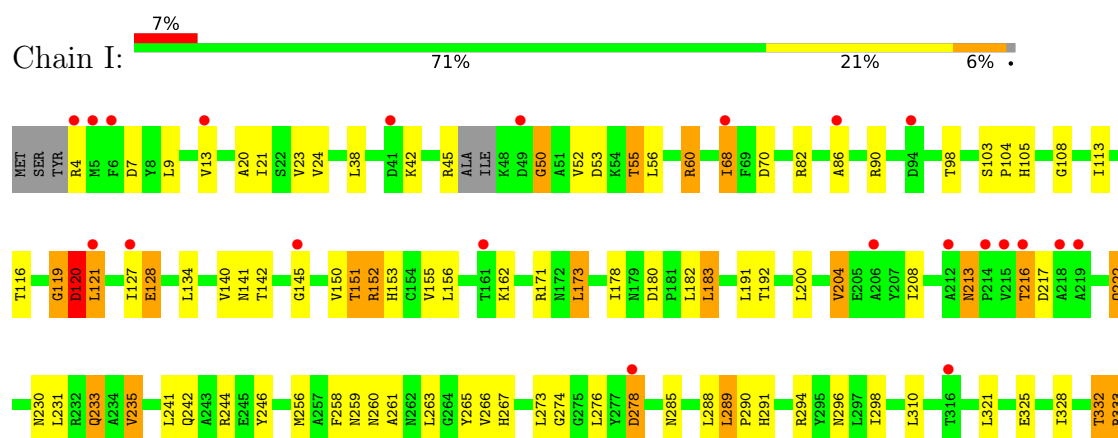
- Molecule 1: 1,3-propanediol oxidoreductase

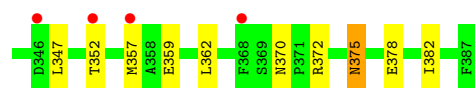


- Molecule 1: 1,3-propanediol oxidoreductase

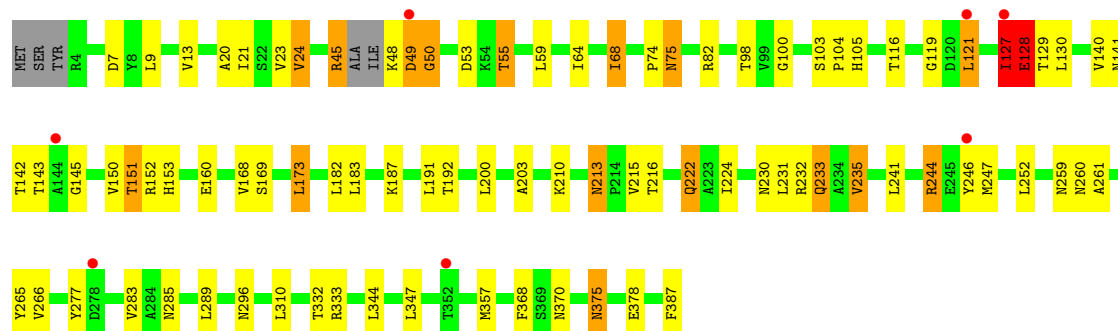
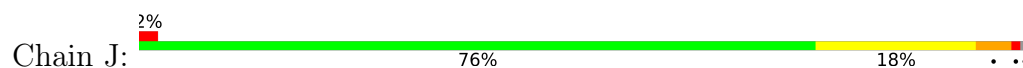


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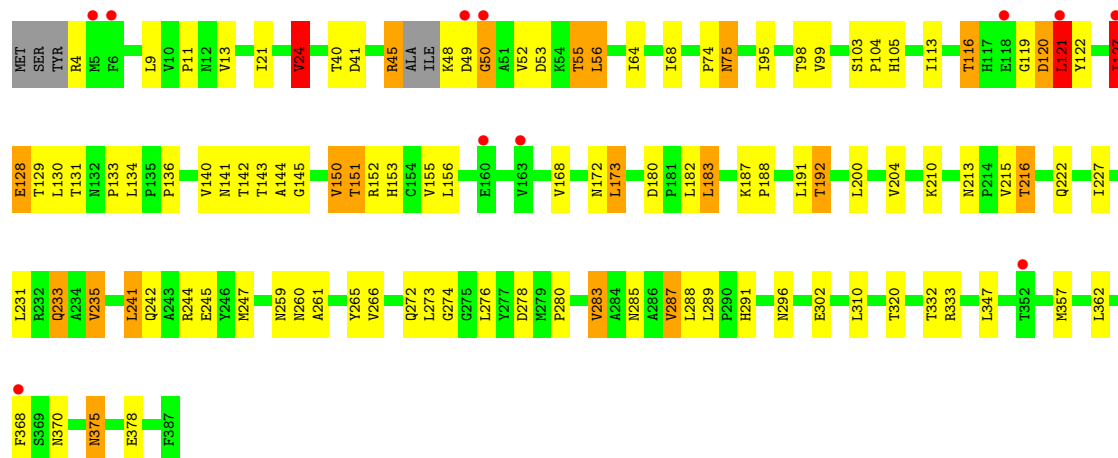




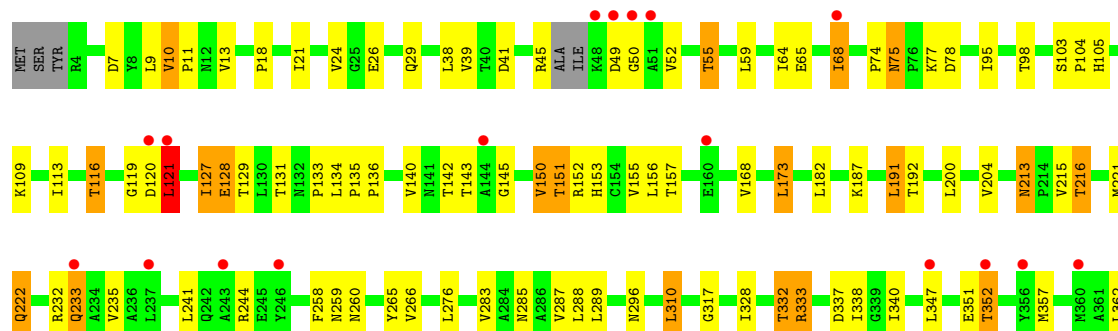
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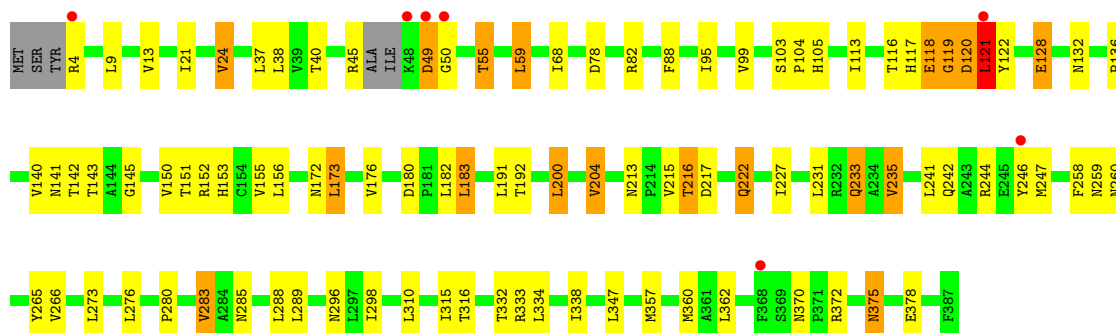
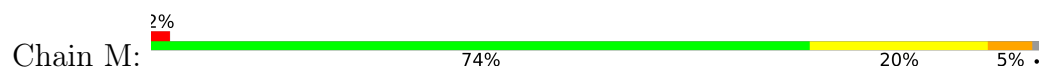


• Molecule 1: 1,3-propanediol oxidoreductase

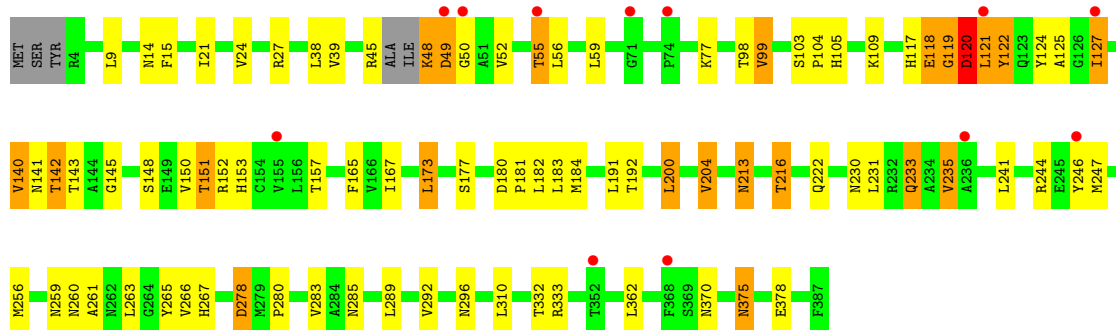
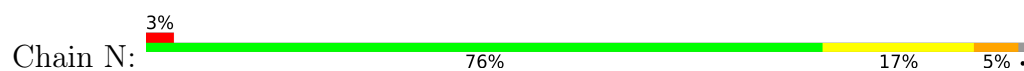




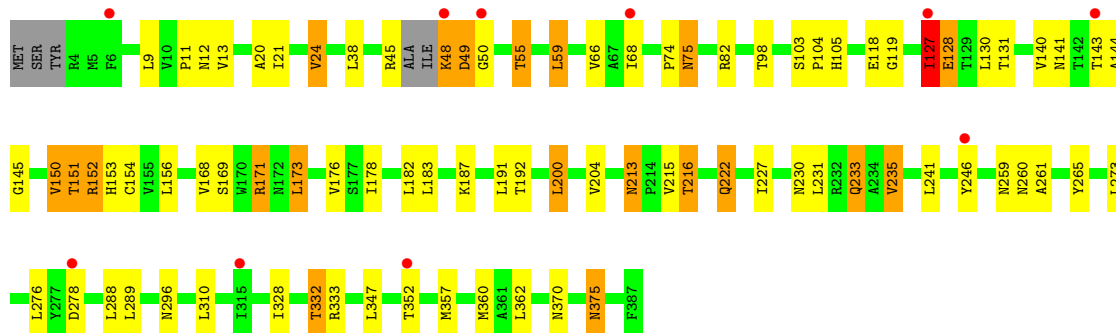
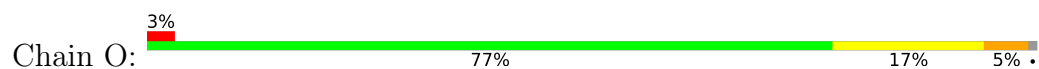
- Molecule 1: 1,3-propanediol oxidoreductase



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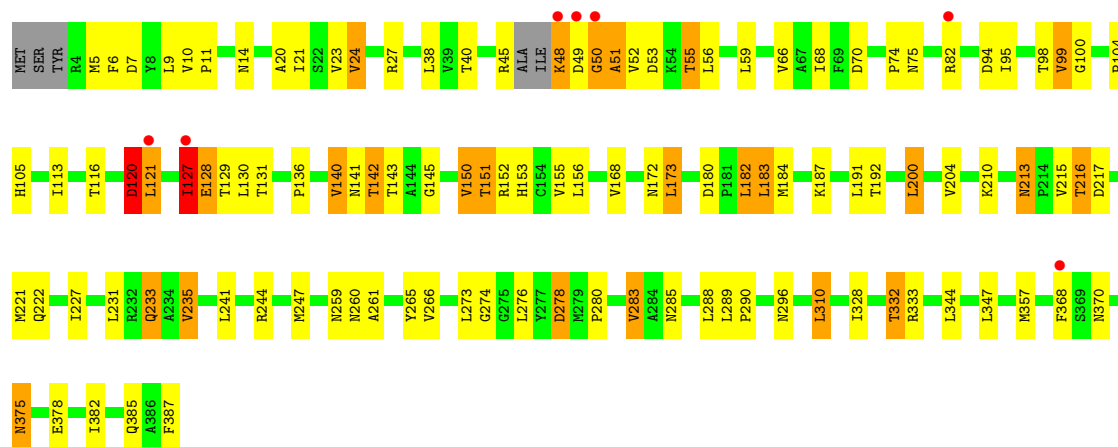


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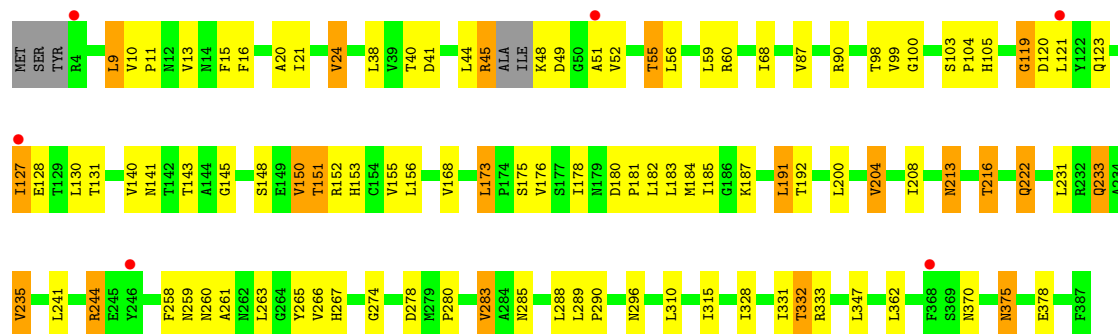
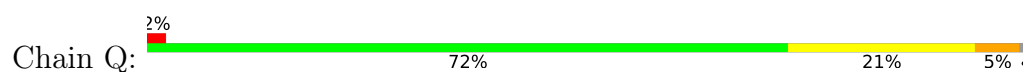


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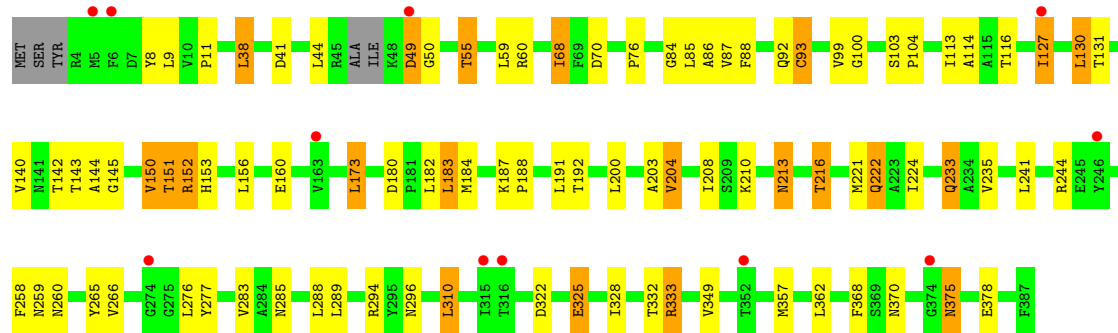
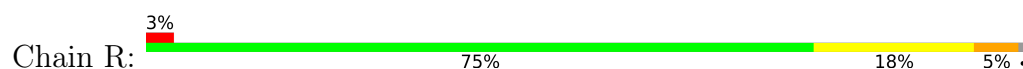




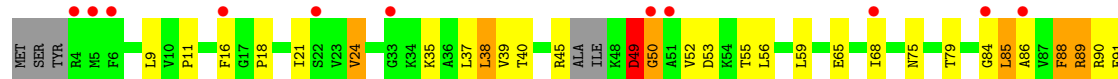
• Molecule 1: 1,3-propanediol oxidoreductase

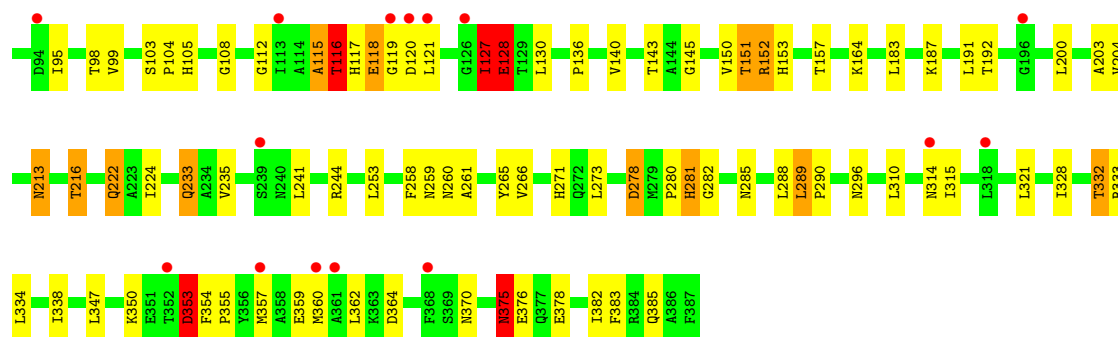


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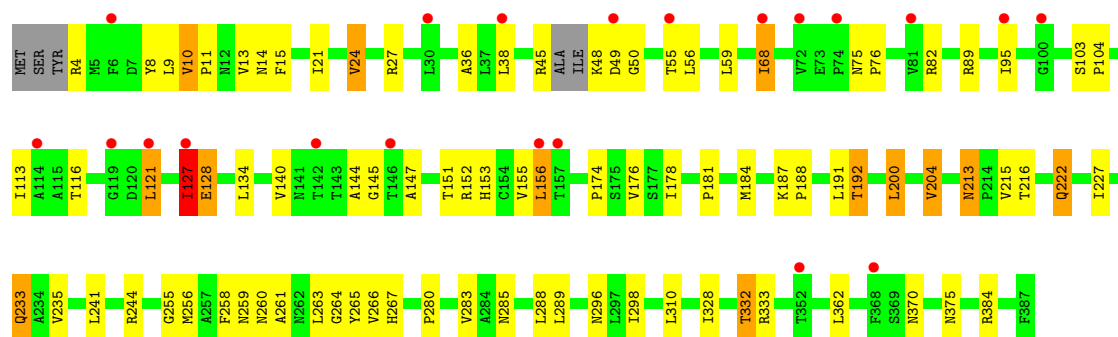
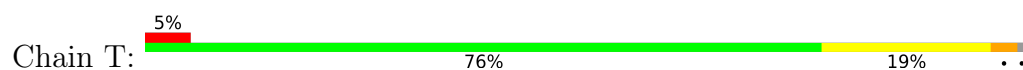


• Molecule 1: 1,3-propanediol oxidoreductase





• Molecule 1: 1,3-propanediol oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.94Å 226.61Å 232.63Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.70) 97.5 (20.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.203 , 0.251 0.198 , 0.243	Depositor DCC
R_{free} test set	12840 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k 0.009 for -h,-l,-k 0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	58348	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 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.50	0/2922	0.85	1/3969 (0.0%)
1	B	0.51	0/2922	0.84	0/3969
1	C	0.49	0/2922	0.83	0/3969
1	D	0.52	0/2922	0.85	1/3969 (0.0%)
1	E	0.58	0/2922	0.90	1/3969 (0.0%)
1	F	0.50	0/2922	0.84	0/3969
1	G	0.56	2/2922 (0.1%)	0.84	1/3969 (0.0%)
1	H	0.54	0/2922	0.91	0/3969
1	I	0.99	7/2922 (0.2%)	0.90	1/3969 (0.0%)
1	J	0.50	0/2922	0.83	0/3969
1	K	0.56	0/2922	0.89	2/3969 (0.1%)
1	L	0.55	2/2922 (0.1%)	0.85	0/3969
1	M	0.52	0/2922	0.87	2/3969 (0.1%)
1	N	0.53	0/2922	0.86	0/3969
1	O	0.52	0/2922	0.87	0/3969
1	P	0.53	0/2922	0.88	0/3969
1	Q	0.51	0/2922	0.86	1/3969 (0.0%)
1	R	0.81	11/2922 (0.4%)	0.88	2/3969 (0.1%)
1	S	1.44	38/2922 (1.3%)	1.14	13/3969 (0.3%)
1	T	0.66	7/2922 (0.2%)	0.90	5/3969 (0.1%)
All	All	0.66	67/58440 (0.1%)	0.88	30/79380 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S	0	3

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	89	ARG	NE-CZ	37.25	1.74	1.33
1	I	60	ARG	CZ-NH1	25.88	1.69	1.32
1	I	90	ARG	NE-CZ	21.31	1.56	1.33
1	S	271	HIS	CG-CD2	20.74	1.58	1.35
1	I	86	ALA	C-N	19.12	1.55	1.33
1	S	89	ARG	CZ-NH2	16.69	1.55	1.33
1	S	271	HIS	CE1-NE2	15.86	1.48	1.32
1	S	115	ALA	C-O	14.42	1.43	1.24
1	S	353	ASP	CG-OD1	14.37	1.52	1.25
1	S	271	HIS	ND1-CE1	13.82	1.46	1.32
1	R	84	GLY	C-O	13.06	1.39	1.23
1	S	353	ASP	C-N	12.70	1.59	1.33
1	T	27	ARG	CZ-NH1	12.30	1.50	1.32
1	S	376	GLU	C-O	12.22	1.38	1.24
1	S	89	ARG	CD-NE	11.49	1.62	1.46
1	I	90	ARG	CZ-NH2	11.13	1.48	1.33
1	R	70	ASP	C-O	11.10	1.39	1.24
1	R	60	ARG	CZ-NH1	11.06	1.48	1.32
1	S	353	ASP	CG-OD2	11.05	1.46	1.25
1	S	271	HIS	CG-ND1	10.63	1.50	1.38
1	S	376	GLU	CD-OE1	9.73	1.43	1.25
1	G	89	ARG	CZ-NH1	9.04	1.45	1.32
1	R	70	ASP	C-N	8.88	1.46	1.33
1	S	383	PHE	CE1-CZ	8.87	1.65	1.38
1	T	27	ARG	NE-CZ	8.79	1.42	1.33
1	I	68	ILE	CB-CG1	8.77	1.71	1.53
1	T	89	ARG	CZ-NH1	8.74	1.45	1.32
1	R	93	CYS	CB-SG	8.67	2.09	1.81
1	L	351	GLU	CD-OE2	8.60	1.41	1.25
1	S	353	ASP	CA-CB	8.58	1.68	1.53
1	I	90	ARG	CD-NE	8.23	1.57	1.46
1	S	89	ARG	CZ-NH1	-8.18	1.21	1.32
1	S	86	ALA	C-N	8.16	1.44	1.33
1	T	27	ARG	CZ-NH2	7.85	1.43	1.33
1	S	383	PHE	CG-CD1	7.83	1.55	1.38
1	S	360	MET	SD-CE	7.81	1.99	1.79
1	I	60	ARG	CD-NE	7.75	1.57	1.46
1	S	116	THR	C-N	7.64	1.43	1.33
1	S	359	GLU	C-O	-7.23	1.15	1.24
1	S	88	PHE	CG-CD1	6.77	1.53	1.38
1	S	85	LEU	CG-CD1	6.77	1.74	1.52
1	S	116	THR	C-O	6.74	1.31	1.24
1	T	27	ARG	CD-NE	6.73	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	86	ALA	C-N	6.32	1.41	1.33
1	T	89	ARG	NE-CZ	6.18	1.39	1.33
1	S	353	ASP	CA-C	6.15	1.61	1.52
1	S	364	ASP	CG-OD2	5.99	1.36	1.25
1	R	87	VAL	C-N	5.98	1.42	1.34
1	T	89	ARG	CZ-NH2	5.73	1.40	1.33
1	S	115	ALA	C-N	5.67	1.41	1.33
1	S	84	GLY	C-O	5.66	1.30	1.23
1	S	116	THR	CA-CB	5.65	1.62	1.53
1	R	86	ALA	C-O	5.61	1.31	1.24
1	L	351	GLU	CD-OE1	5.60	1.35	1.25
1	S	84	GLY	C-N	5.58	1.41	1.34
1	S	89	ARG	CG-CD	5.48	1.68	1.52
1	S	278	ASP	CG-OD2	5.44	1.35	1.25
1	S	376	GLU	C-N	5.41	1.41	1.33
1	R	84	GLY	C-N	5.38	1.41	1.33
1	S	88	PHE	CA-C	5.37	1.59	1.52
1	R	60	ARG	NE-CZ	5.35	1.39	1.33
1	S	91	GLU	CD-OE2	5.24	1.35	1.25
1	R	92	GLN	CD-OE1	5.23	1.33	1.23
1	G	89	ARG	CZ-NH2	5.16	1.40	1.33
1	S	112	GLY	C-O	5.11	1.29	1.23
1	S	91	GLU	CD-OE1	5.05	1.34	1.25
1	S	383	PHE	CG-CD2	5.03	1.49	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	89	ARG	NE-CZ-NH2	-25.54	96.21	119.20
1	S	89	ARG	NH1-CZ-NH2	19.91	145.18	119.30
1	S	89	ARG	CD-NE-CZ	-16.68	101.05	124.40
1	T	27	ARG	NE-CZ-NH2	-11.58	108.78	119.20
1	I	90	ARG	NE-CZ-NH2	-10.10	110.11	119.20
1	S	271	HIS	ND1-CE1-NE2	9.42	117.82	108.40
1	S	353	ASP	O-C-N	8.92	134.46	122.59
1	S	89	ARG	CG-CD-NE	-7.88	94.67	112.00
1	T	27	ARG	CD-NE-CZ	-7.84	113.42	124.40
1	T	89	ARG	NE-CZ-NH2	-7.72	112.25	119.20
1	S	271	HIS	CG-ND1-CE1	-7.14	97.16	109.30
1	S	271	HIS	CB-CG-ND1	-6.92	112.32	122.70
1	G	89	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	S	375	ASN	OD1-CG-ND2	6.47	129.07	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	ASP	N-CA-C	6.19	116.03	107.73
1	K	40	THR	N-CA-C	5.88	116.31	108.38
1	R	60	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	S	271	HIS	ND1-CG-CD2	5.53	111.63	106.10
1	S	90	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	T	89	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	K	24	VAL	N-CA-CB	5.30	116.39	110.51
1	M	40	THR	N-CA-C	5.29	115.53	108.38
1	T	27	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	S	86	ALA	O-C-N	5.21	128.68	122.27
1	R	87	VAL	N-CA-C	-5.19	106.08	111.58
1	S	40	THR	N-CA-C	5.17	114.96	108.45
1	A	40	THR	N-CA-C	5.11	114.89	108.45
1	Q	40	THR	N-CA-C	5.10	115.27	108.38
1	M	316	THR	N-CA-C	5.09	116.52	110.97
1	D	316	THR	N-CA-C	5.03	117.16	111.02

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S	116	THR	Mainchain
1	S	353	ASP	Sidechain,Mainchain

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	2871	0	2872	61	0
1	B	2871	0	2872	62	0
1	C	2871	0	2872	53	0
1	D	2871	0	2872	55	0
1	E	2871	0	2872	50	0
1	F	2871	0	2872	51	0
1	G	2871	0	2872	59	0
1	H	2871	0	2872	82	0
1	I	2871	0	2872	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2871	0	2872	49	0
1	K	2871	0	2872	67	0
1	L	2871	0	2872	56	0
1	M	2871	0	2872	56	0
1	N	2871	0	2872	57	0
1	O	2871	0	2872	54	0
1	P	2871	0	2872	68	0
1	Q	2871	0	2872	51	0
1	R	2871	0	2872	50	0
1	S	2871	0	2872	69	0
1	T	2871	0	2872	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	36	0	0	3	0
3	B	45	0	0	4	0
3	C	27	0	0	3	0
3	D	49	0	0	6	0
3	E	76	0	0	3	0
3	F	19	0	0	2	0
3	G	41	0	0	1	0
3	H	61	0	0	8	0
3	I	51	0	0	6	0
3	J	31	0	0	2	0
3	K	89	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	42	0	0	0	0
3	M	58	0	0	1	0
3	N	33	0	0	2	0
3	O	50	0	0	3	0
3	P	64	0	0	5	0
3	Q	43	0	0	1	0
3	R	39	0	0	0	0
3	S	19	0	0	6	0
3	T	35	0	0	1	0
All	All	58348	0	57440	1128	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 10.

All (1128) 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:S:85:LEU:CG	1:S:85:LEU:CD1	1.74	1.63
1:I:60:ARG:CZ	1:I:60:ARG:NH1	1.69	1.52
1:S:89:ARG:NE	1:S:89:ARG:CZ	1.74	1.49
1:R:93:CYS:CB	1:R:93:CYS:SG	2.09	1.39
1:H:171:ARG:HG2	1:H:171:ARG:HH11	1.16	1.05
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.28	0.97
1:C:233:GLN:H	1:C:233:GLN:HE21	1.11	0.96
1:T:216:THR:HG21	1:T:261:ALA:HB2	1.47	0.96
1:H:233:GLN:H	1:H:233:GLN:HE21	0.97	0.95
1:D:216:THR:HG22	3:D:1429:HOH:O	1.66	0.95
1:N:233:GLN:H	1:N:233:GLN:HE21	1.15	0.94
1:J:233:GLN:H	1:J:233:GLN:HE21	1.11	0.94
1:G:233:GLN:H	1:G:233:GLN:HE21	1.04	0.94
1:E:9:LEU:H	1:E:260:ASN:HD21	1.16	0.93
1:E:21:ILE:O	1:E:24:VAL:HG23	1.69	0.93
1:M:233:GLN:H	1:M:233:GLN:HE21	1.17	0.93
1:O:233:GLN:H	1:O:233:GLN:HE21	1.12	0.91
1:O:9:LEU:H	1:O:260:ASN:HD21	1.17	0.91
1:A:233:GLN:H	1:A:233:GLN:HE21	1.18	0.91
1:D:233:GLN:H	1:D:233:GLN:HE21	1.16	0.91
1:L:233:GLN:H	1:L:233:GLN:HE21	1.11	0.91
1:K:233:GLN:HE21	1:K:233:GLN:H	0.97	0.90
1:E:233:GLN:H	1:E:233:GLN:HE21	1.16	0.89
1:Q:233:GLN:H	1:Q:233:GLN:HE21	1.15	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:9:LEU:H	1:K:260:ASN:HD21	1.18	0.89
1:E:9:LEU:H	1:E:260:ASN:ND2	1.71	0.88
1:P:9:LEU:H	1:P:260:ASN:HD21	1.23	0.87
1:E:82:ARG:HB3	3:E:1462:HOH:O	1.74	0.85
1:K:233:GLN:HE21	1:K:233:GLN:N	1.76	0.84
1:I:119:GLY:O	1:I:120:ASP:HB2	1.78	0.84
1:B:9:LEU:H	1:B:260:ASN:HD21	1.23	0.83
1:J:216:THR:HG21	1:J:261:ALA:HB2	1.61	0.83
1:M:152:ARG:H	1:M:259:ASN:HD21	1.26	0.83
1:T:233:GLN:H	1:T:233:GLN:HE21	1.26	0.83
1:P:233:GLN:HE21	1:P:233:GLN:H	1.26	0.83
1:B:233:GLN:H	1:B:233:GLN:HE21	1.25	0.83
1:G:216:THR:HG21	1:G:261:ALA:HB2	1.60	0.83
1:J:21:ILE:O	1:J:24:VAL:HG22	1.80	0.82
1:I:256:MET:HE3	3:I:1435:HOH:O	1.79	0.82
1:M:151:THR:HG22	1:M:153:HIS:H	1.42	0.82
1:O:152:ARG:H	1:O:259:ASN:HD21	1.27	0.82
1:B:9:LEU:H	1:B:260:ASN:ND2	1.78	0.81
1:O:9:LEU:H	1:O:260:ASN:ND2	1.77	0.81
1:F:9:LEU:H	1:F:260:ASN:ND2	1.78	0.81
1:R:296:ASN:HD21	1:R:370:ASN:HD21	1.25	0.81
1:C:233:GLN:HE21	1:C:233:GLN:N	1.79	0.80
1:H:233:GLN:H	1:H:233:GLN:NE2	1.76	0.80
1:C:9:LEU:H	1:C:260:ASN:ND2	1.79	0.80
1:E:151:THR:HG23	1:E:153:HIS:H	1.46	0.80
1:S:89:ARG:CZ	1:S:89:ARG:CD	2.59	0.80
1:H:233:GLN:HE21	1:H:233:GLN:N	1.78	0.79
1:K:9:LEU:H	1:K:260:ASN:ND2	1.80	0.79
1:A:328:ILE:O	1:A:332:THR:HG22	1.81	0.78
1:S:233:GLN:H	1:S:233:GLN:HE21	1.29	0.78
1:H:9:LEU:H	1:H:260:ASN:HD21	1.30	0.78
1:Q:60:ARG:HG3	1:Q:60:ARG:HH11	1.48	0.78
1:K:273:LEU:HD23	1:K:357:MET:HE1	1.65	0.78
1:C:216:THR:HG21	1:C:261:ALA:HB2	1.65	0.78
1:N:151:THR:HG23	1:N:153:HIS:H	1.47	0.78
1:R:233:GLN:H	1:R:233:GLN:HE21	1.31	0.77
1:H:9:LEU:H	1:H:260:ASN:ND2	1.82	0.77
1:A:9:LEU:H	1:A:260:ASN:HD21	1.30	0.77
1:K:296:ASN:HD21	1:K:370:ASN:HD21	1.33	0.77
1:F:233:GLN:H	1:F:233:GLN:HE21	1.33	0.77
1:I:171:ARG:HG2	1:I:171:ARG:HH11	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:328:ILE:O	1:O:332:THR:HG22	1.86	0.76
1:S:117:HIS:HB3	3:S:1390:HOH:O	1.84	0.76
1:D:119:GLY:O	1:D:120:ASP:HB2	1.86	0.76
1:M:9:LEU:HB3	1:M:173:LEU:HD21	1.68	0.76
1:S:204:VAL:HG21	1:S:289:LEU:HD21	1.67	0.76
1:D:216:THR:HG21	1:D:261:ALA:HB2	1.68	0.76
1:H:171:ARG:HH11	1:H:171:ARG:CG	1.97	0.76
1:I:233:GLN:H	1:I:233:GLN:HE21	1.33	0.76
1:C:9:LEU:H	1:C:260:ASN:HD21	1.29	0.75
1:R:152:ARG:H	1:R:259:ASN:HD21	1.34	0.75
1:D:222:GLN:HE21	1:D:222:GLN:HA	1.51	0.75
1:D:9:LEU:H	1:D:260:ASN:HD21	1.31	0.75
1:F:280:PRO:HB2	1:F:283:VAL:HG12	1.67	0.75
1:H:296:ASN:HD21	1:H:370:ASN:HD21	1.35	0.75
1:Q:9:LEU:H	1:Q:260:ASN:HD21	1.35	0.75
1:O:171:ARG:HH11	1:O:171:ARG:HG2	1.52	0.75
1:D:9:LEU:H	1:D:260:ASN:ND2	1.83	0.74
1:M:9:LEU:H	1:M:260:ASN:HD21	1.35	0.74
1:B:119:GLY:O	1:B:120:ASP:HB2	1.84	0.74
1:K:21:ILE:O	1:K:24:VAL:HG22	1.88	0.74
1:N:9:LEU:H	1:N:260:ASN:HD21	1.35	0.74
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.00	0.74
1:T:151:THR:HG22	1:T:153:HIS:H	1.51	0.73
1:E:152:ARG:H	1:E:259:ASN:HD21	1.35	0.73
3:J:1418:HOH:O	1:N:256:MET:HE3	1.87	0.73
1:S:103:SER:HB2	1:S:104:PRO:HD3	1.70	0.73
1:L:276:LEU:HD12	1:L:357:MET:HE3	1.69	0.73
1:G:9:LEU:H	1:G:260:ASN:HD21	1.33	0.73
1:G:233:GLN:H	1:G:233:GLN:NE2	1.85	0.73
1:N:105:HIS:HE1	1:N:141:ASN:HD22	1.36	0.73
1:C:151:THR:HG22	1:C:153:HIS:H	1.53	0.73
1:F:296:ASN:HD21	1:F:370:ASN:HD21	1.33	0.73
1:F:9:LEU:H	1:F:260:ASN:HD21	1.37	0.73
1:H:216:THR:HG21	1:H:261:ALA:HB2	1.71	0.73
1:H:256:MET:HE3	3:H:1393:HOH:O	1.89	0.72
1:I:291:HIS:HD2	3:I:1415:HOH:O	1.72	0.72
1:I:296:ASN:HD21	1:I:370:ASN:HD21	1.38	0.72
1:J:152:ARG:H	1:J:259:ASN:HD21	1.36	0.72
1:S:9:LEU:H	1:S:260:ASN:ND2	1.86	0.72
1:T:328:ILE:O	1:T:332:THR:HG22	1.90	0.72
1:O:171:ARG:HH11	1:O:171:ARG:CG	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:THR:HG22	3:C:1400:HOH:O	1.88	0.72
1:E:277:TYR:HE2	1:E:357:MET:HE1	1.53	0.72
1:M:9:LEU:H	1:M:260:ASN:ND2	1.86	0.72
1:F:121:LEU:HG	1:F:122:TYR:H	1.54	0.72
1:K:21:ILE:HD11	1:K:55:THR:HB	1.72	0.72
1:A:151:THR:HG23	1:A:153:HIS:H	1.53	0.72
1:P:276:LEU:HD12	1:P:357:MET:HE3	1.71	0.71
1:B:9:LEU:HB3	1:B:173:LEU:HD21	1.71	0.71
1:R:222:GLN:HA	1:R:222:GLN:HE21	1.55	0.71
1:S:85:LEU:CD1	1:S:85:LEU:CB	2.68	0.71
1:P:9:LEU:H	1:P:260:ASN:ND2	1.87	0.71
1:G:368:PHE:HB2	3:G:1428:HOH:O	1.91	0.71
1:B:368:PHE:HB2	3:B:1400:HOH:O	1.90	0.71
1:D:60:ARG:HG3	1:D:60:ARG:HH11	1.55	0.71
1:F:151:THR:HG23	1:F:153:HIS:H	1.55	0.71
1:J:9:LEU:H	1:J:260:ASN:ND2	1.89	0.71
1:D:266:VAL:HG12	1:D:285:ASN:HD22	1.55	0.70
1:L:151:THR:HG23	1:L:153:HIS:H	1.55	0.70
1:O:21:ILE:O	1:O:24:VAL:HG22	1.91	0.70
1:T:152:ARG:H	1:T:259:ASN:HD21	1.37	0.70
1:A:9:LEU:H	1:A:260:ASN:ND2	1.90	0.70
1:G:9:LEU:H	1:G:260:ASN:ND2	1.88	0.70
1:J:45:ARG:HH21	1:J:68:ILE:HD11	1.57	0.70
1:M:273:LEU:HD23	1:M:357:MET:HE1	1.73	0.70
1:J:98:THR:OG1	1:J:105:HIS:HD2	1.74	0.69
1:J:9:LEU:H	1:J:260:ASN:HD21	1.38	0.69
1:G:233:GLN:HE21	1:G:233:GLN:N	1.84	0.69
1:K:291:HIS:HD2	3:K:1447:HOH:O	1.75	0.69
1:E:152:ARG:H	1:E:259:ASN:ND2	1.90	0.69
1:F:273:LEU:HD23	1:F:357:MET:HE1	1.75	0.69
1:H:171:ARG:HG2	1:H:171:ARG:NH1	1.97	0.69
1:N:9:LEU:H	1:N:260:ASN:ND2	1.90	0.69
1:Q:328:ILE:O	1:Q:332:THR:HG22	1.93	0.69
1:K:152:ARG:H	1:K:259:ASN:HD21	1.39	0.69
1:J:265:TYR:H	1:J:370:ASN:ND2	1.91	0.68
1:L:266:VAL:HG12	1:L:285:ASN:HD22	1.57	0.68
1:A:213:ASN:ND2	1:A:216:THR:H	1.91	0.68
1:J:233:GLN:HE21	1:J:233:GLN:N	1.90	0.68
1:H:9:LEU:HB3	1:H:173:LEU:HD21	1.73	0.68
1:P:121:LEU:HA	3:P:1449:HOH:O	1.93	0.68
1:Q:266:VAL:HG12	1:Q:285:ASN:HD22	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:213:ASN:ND2	1:S:216:THR:H	1.91	0.68
1:N:230:ASN:OD1	1:N:246:TYR:HD2	1.75	0.68
1:G:121:LEU:HD23	1:G:121:LEU:H	1.58	0.68
1:M:128:GLU:HG3	3:M:1400:HOH:O	1.93	0.68
1:E:233:GLN:H	1:E:233:GLN:NE2	1.90	0.68
1:E:276:LEU:HD12	1:E:357:MET:HE3	1.75	0.68
1:H:266:VAL:HG12	1:H:285:ASN:HD22	1.58	0.68
1:L:233:GLN:HE21	1:L:233:GLN:N	1.90	0.68
1:A:8:TYR:CE2	1:D:256:MET:HE1	2.28	0.67
1:A:21:ILE:O	1:A:24:VAL:HG23	1.94	0.67
1:D:265:TYR:H	1:D:370:ASN:ND2	1.92	0.67
1:F:152:ARG:H	1:F:259:ASN:HD21	1.42	0.67
1:L:152:ARG:H	1:L:259:ASN:HD21	1.39	0.67
1:R:9:LEU:H	1:R:260:ASN:ND2	1.92	0.67
1:G:328:ILE:O	1:G:332:THR:HG22	1.95	0.67
1:A:105:HIS:HE1	1:A:141:ASN:HD22	1.42	0.67
1:G:213:ASN:ND2	1:G:216:THR:H	1.93	0.67
1:L:103:SER:HB2	1:L:104:PRO:HD3	1.77	0.67
1:Q:152:ARG:H	1:Q:259:ASN:HD21	1.42	0.67
1:F:9:LEU:HB3	1:F:173:LEU:HD21	1.74	0.67
1:K:9:LEU:HB3	1:K:173:LEU:HD21	1.76	0.67
1:N:233:GLN:H	1:N:233:GLN:NE2	1.91	0.67
1:P:21:ILE:O	1:P:24:VAL:HG22	1.94	0.67
1:H:152:ARG:H	1:H:259:ASN:HD21	1.43	0.67
1:B:151:THR:HG23	1:B:153:HIS:H	1.59	0.66
1:I:105:HIS:HE1	1:I:141:ASN:HD22	1.43	0.66
1:E:45:ARG:C	1:E:48:LYS:HE3	2.20	0.66
1:M:103:SER:HB2	1:M:104:PRO:HD3	1.78	0.66
1:N:296:ASN:HD21	1:N:370:ASN:HD21	1.43	0.66
1:B:283:VAL:O	1:B:287:VAL:HG12	1.95	0.66
1:M:296:ASN:HD21	1:M:370:ASN:HD21	1.43	0.66
1:B:296:ASN:HD21	1:B:370:ASN:HD21	1.43	0.66
1:K:233:GLN:H	1:K:233:GLN:NE2	1.82	0.66
1:R:9:LEU:H	1:R:260:ASN:HD21	1.44	0.66
1:Q:222:GLN:HA	1:Q:222:GLN:HE21	1.60	0.66
1:E:277:TYR:CE2	1:E:357:MET:HE1	2.30	0.66
1:L:13:VAL:HG22	1:M:9:LEU:HD22	1.77	0.65
1:H:151:THR:HG22	1:H:153:HIS:H	1.62	0.65
1:I:375:ASN:C	1:I:375:ASN:HD22	2.04	0.65
1:K:152:ARG:H	1:K:259:ASN:ND2	1.94	0.65
1:P:27:ARG:HD3	3:P:1406:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:151:THR:HG22	1:R:153:HIS:H	1.62	0.65
1:O:233:GLN:H	1:O:233:GLN:NE2	1.91	0.65
1:G:152:ARG:H	1:G:259:ASN:HD21	1.44	0.65
1:O:273:LEU:HD23	1:O:357:MET:HE1	1.79	0.65
1:P:296:ASN:HD21	1:P:370:ASN:HD21	1.43	0.65
1:T:233:GLN:H	1:T:233:GLN:NE2	1.95	0.65
1:G:52:VAL:HG12	1:G:99:VAL:HG21	1.79	0.65
1:O:216:THR:CG2	3:O:1436:HOH:O	2.45	0.65
1:H:121:LEU:HG	1:H:122:TYR:H	1.62	0.64
1:C:21:ILE:HD11	1:C:55:THR:HB	1.77	0.64
1:L:9:LEU:H	1:L:260:ASN:HD21	1.46	0.64
1:P:265:TYR:H	1:P:370:ASN:ND2	1.96	0.64
1:H:45:ARG:O	1:H:48:LYS:N	2.31	0.64
1:L:152:ARG:H	1:L:259:ASN:ND2	1.95	0.64
1:P:7:ASP:HB3	1:Q:15:PHE:CE2	2.32	0.64
1:I:180:ASP:HB3	1:I:183:LEU:HD22	1.79	0.64
1:S:89:ARG:NE	1:S:89:ARG:NH2	2.45	0.64
1:I:21:ILE:O	1:I:24:VAL:HG23	1.98	0.64
1:O:216:THR:HG21	1:O:261:ALA:HB2	1.79	0.63
1:A:78:ASP:HB2	1:A:121:LEU:HD13	1.80	0.63
1:O:151:THR:HG23	1:O:153:HIS:H	1.63	0.63
1:P:51:ALA:HB3	3:P:1394:HOH:O	1.98	0.63
1:R:266:VAL:HG12	1:R:285:ASN:HD22	1.63	0.63
1:D:60:ARG:HH11	1:D:60:ARG:CG	2.11	0.63
1:I:4:ARG:N	3:I:1393:HOH:O	2.30	0.63
1:L:9:LEU:H	1:L:260:ASN:ND2	1.96	0.63
1:N:231:LEU:O	1:N:235:VAL:HG13	1.98	0.63
1:O:213:ASN:ND2	1:O:216:THR:H	1.96	0.63
1:N:103:SER:HB2	1:N:104:PRO:HD3	1.79	0.63
1:T:82:ARG:HH22	1:T:121:LEU:HD22	1.63	0.63
1:C:216:THR:CG2	3:C:1400:HOH:O	2.45	0.63
1:P:290:PRO:HB3	1:P:332:THR:HG22	1.79	0.63
1:C:152:ARG:H	1:C:259:ASN:HD21	1.47	0.62
1:J:265:TYR:H	1:J:370:ASN:HD22	1.46	0.62
1:Q:9:LEU:H	1:Q:260:ASN:ND2	1.96	0.62
1:Q:213:ASN:ND2	1:Q:216:THR:H	1.97	0.62
1:D:27:ARG:HD3	3:D:1393:HOH:O	1.99	0.62
1:P:274:GLY:O	1:P:278:ASP:HA	1.99	0.62
1:R:103:SER:HB2	1:R:104:PRO:HD3	1.82	0.62
1:A:233:GLN:HE21	1:A:233:GLN:N	1.95	0.62
1:E:180:ASP:HB3	1:E:183:LEU:HD22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:LEU:HD12	1:F:357:MET:HE3	1.80	0.62
1:K:105:HIS:HE1	1:K:141:ASN:HD22	1.47	0.62
1:M:233:GLN:H	1:M:233:GLN:NE2	1.93	0.62
1:N:213:ASN:ND2	1:N:216:THR:H	1.97	0.62
1:O:153:HIS:HD2	1:O:168:VAL:HG22	1.64	0.62
1:D:152:ARG:H	1:D:259:ASN:HD21	1.47	0.62
1:E:98:THR:OG1	1:E:105:HIS:HD2	1.82	0.62
1:D:180:ASP:HB3	1:D:183:LEU:HD22	1.80	0.62
1:K:375:ASN:C	1:K:375:ASN:HD22	2.08	0.62
1:P:233:GLN:HE21	1:P:233:GLN:N	1.98	0.62
1:S:21:ILE:O	1:S:24:VAL:HG22	2.00	0.62
1:G:55:THR:HG21	1:G:99:VAL:HG11	1.82	0.62
1:D:21:ILE:O	1:D:24:VAL:HG22	2.00	0.62
1:G:283:VAL:O	1:G:287:VAL:HG12	1.99	0.62
1:E:121:LEU:HB2	3:E:1404:HOH:O	1.98	0.62
1:O:265:TYR:H	1:O:370:ASN:ND2	1.98	0.62
1:M:119:GLY:O	1:M:120:ASP:HB2	2.00	0.61
1:T:213:ASN:ND2	1:T:216:THR:H	1.98	0.61
1:C:328:ILE:O	1:C:332:THR:HG22	2.00	0.61
1:J:216:THR:HG21	1:J:261:ALA:CB	2.30	0.61
1:M:82:ARG:NH1	1:M:121:LEU:HD21	2.14	0.61
1:A:119:GLY:O	1:A:120:ASP:HB2	1.98	0.61
1:G:152:ARG:H	1:G:259:ASN:ND2	1.99	0.61
1:P:265:TYR:H	1:P:370:ASN:HD22	1.49	0.61
1:S:85:LEU:CD1	1:S:85:LEU:CD2	2.75	0.61
1:D:231:LEU:O	1:D:235:VAL:HG13	2.00	0.61
1:J:213:ASN:ND2	1:J:216:THR:H	1.99	0.61
1:R:11:PRO:HD2	1:R:150:VAL:HG22	1.83	0.61
1:G:276:LEU:HD12	1:G:357:MET:HE3	1.83	0.61
1:J:230:ASN:OD1	1:J:246:TYR:HD2	1.83	0.61
1:Q:265:TYR:H	1:Q:370:ASN:ND2	1.97	0.61
1:J:231:LEU:O	1:J:235:VAL:HG13	2.00	0.61
1:O:152:ARG:H	1:O:259:ASN:ND2	1.97	0.61
1:C:204:VAL:HG21	1:C:289:LEU:HD21	1.83	0.61
1:T:266:VAL:HG12	1:T:285:ASN:HD22	1.64	0.61
1:K:103:SER:HB2	1:K:104:PRO:HD3	1.81	0.61
1:Q:187:LYS:HD2	1:Q:191:LEU:HD12	1.82	0.61
1:Q:233:GLN:HE21	1:Q:233:GLN:N	1.94	0.61
1:E:222:GLN:HE21	1:E:222:GLN:HA	1.66	0.60
1:G:103:SER:HB2	1:G:104:PRO:HD3	1.83	0.60
1:G:105:HIS:HE1	1:G:141:ASN:HD22	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:VAL:HG12	1:I:285:ASN:HD22	1.65	0.60
1:P:82:ARG:HD2	3:P:1399:HOH:O	2.00	0.60
1:S:273:LEU:HD23	1:S:357:MET:HE1	1.83	0.60
1:C:276:LEU:HD12	1:C:357:MET:HE3	1.83	0.60
1:D:265:TYR:H	1:D:370:ASN:HD22	1.49	0.60
1:J:222:GLN:HA	1:J:222:GLN:HE21	1.65	0.60
1:M:200:LEU:O	1:M:204:VAL:HG13	2.01	0.60
1:R:265:TYR:H	1:R:370:ASN:ND2	1.99	0.60
1:I:273:LEU:HD23	1:I:357:MET:HE1	1.82	0.60
1:L:9:LEU:HD22	1:M:13:VAL:HG22	1.81	0.60
1:A:242:GLN:HE21	1:A:246:TYR:HE2	1.50	0.60
1:R:55:THR:O	1:R:59:LEU:HB2	2.02	0.60
1:S:354:PHE:N	1:S:355:PRO:CD	2.64	0.60
1:N:280:PRO:HB2	1:N:283:VAL:HG22	1.84	0.60
1:D:152:ARG:H	1:D:259:ASN:ND2	2.00	0.60
1:I:9:LEU:H	1:I:260:ASN:ND2	2.00	0.60
1:R:213:ASN:ND2	1:R:216:THR:H	1.99	0.60
1:F:329:ALA:HA	1:F:332:THR:HG22	1.84	0.60
1:K:45:ARG:O	1:K:48:LYS:N	2.35	0.60
1:K:151:THR:HG23	1:K:153:HIS:H	1.66	0.60
1:R:276:LEU:HD12	1:R:357:MET:HE3	1.83	0.59
1:D:216:THR:HG21	1:D:261:ALA:CB	2.32	0.59
1:E:121:LEU:HD23	1:E:122:TYR:H	1.67	0.59
1:I:24:VAL:HG22	1:I:178:ILE:HD13	1.82	0.59
1:B:103:SER:HB2	1:B:104:PRO:HD3	1.83	0.59
1:J:266:VAL:HG12	1:J:285:ASN:HD22	1.67	0.59
1:L:382:ILE:HA	1:L:385:GLN:HE21	1.66	0.59
1:P:213:ASN:ND2	1:P:216:THR:H	2.00	0.59
1:D:146:THR:HG22	1:D:148:SER:H	1.67	0.59
1:G:362:LEU:HD12	1:G:376:GLU:HG3	1.83	0.59
1:O:49:ASP:N	1:O:49:ASP:OD1	2.36	0.59
1:L:9:LEU:HB3	1:L:173:LEU:HD21	1.83	0.59
1:L:26:GLU:HA	1:L:29:GLN:HE21	1.66	0.59
1:C:45:ARG:C	1:C:48:LYS:N	2.61	0.59
1:M:152:ARG:H	1:M:259:ASN:ND2	1.97	0.59
1:H:9:LEU:HD22	1:K:13:VAL:HG22	1.85	0.59
1:R:151:THR:CG2	1:R:153:HIS:H	2.16	0.59
1:A:171:ARG:HG2	1:A:171:ARG:NH1	2.09	0.58
1:L:187:LYS:HD2	1:L:191:LEU:HD13	1.84	0.58
1:O:296:ASN:HD21	1:O:370:ASN:HD21	1.51	0.58
1:Q:21:ILE:O	1:Q:24:VAL:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:213:ASN:ND2	1:H:216:THR:H	2.00	0.58
1:P:152:ARG:H	1:P:259:ASN:HD21	1.50	0.58
1:H:216:THR:CG2	3:H:1429:HOH:O	2.51	0.58
1:Q:105:HIS:HE1	1:Q:141:ASN:HD22	1.50	0.58
1:F:100:GLY:HA3	1:F:104:PRO:HG2	1.84	0.58
1:B:328:ILE:O	1:B:332:THR:HG22	2.03	0.58
1:Q:151:THR:HG23	1:Q:153:HIS:H	1.68	0.58
1:F:200:LEU:HG	1:F:227:ILE:HG21	1.85	0.58
1:R:294:ARG:NH1	1:R:328:ILE:HG21	2.18	0.58
1:B:276:LEU:HD12	1:B:357:MET:HE3	1.85	0.58
1:D:9:LEU:HB3	1:D:173:LEU:HD21	1.85	0.58
1:I:9:LEU:HB3	1:I:173:LEU:HD21	1.84	0.58
1:I:213:ASN:ND2	1:I:216:THR:H	2.02	0.58
1:I:230:ASN:OD1	1:I:246:TYR:HD2	1.87	0.58
1:O:233:GLN:HE21	1:O:233:GLN:N	1.94	0.58
1:M:360:MET:HA	1:M:360:MET:HE2	1.85	0.58
1:R:296:ASN:HD21	1:R:370:ASN:ND2	1.99	0.58
1:C:296:ASN:HD21	1:C:370:ASN:HD21	1.52	0.58
1:K:216:THR:HG21	1:K:261:ALA:HB2	1.85	0.58
1:B:213:ASN:ND2	1:B:216:THR:H	2.03	0.57
1:Q:153:HIS:HD2	1:Q:168:VAL:HG22	1.68	0.57
1:L:74:PRO:O	1:L:75:ASN:HB2	2.03	0.57
1:N:48:LYS:HD2	1:N:49:ASP:OD1	2.04	0.57
1:I:233:GLN:HE21	1:I:233:GLN:N	2.02	0.57
1:B:82:ARG:HB3	3:B:1397:HOH:O	2.04	0.57
1:H:105:HIS:HE1	1:H:141:ASN:HD22	1.51	0.57
1:N:9:LEU:HB3	1:N:173:LEU:HD21	1.86	0.57
1:O:216:THR:HG23	3:O:1436:HOH:O	2.04	0.57
1:Q:296:ASN:HD21	1:Q:370:ASN:HD21	1.52	0.57
1:E:105:HIS:HE1	1:E:141:ASN:HD22	1.52	0.57
1:G:151:THR:HG23	1:G:153:HIS:H	1.69	0.57
1:B:74:PRO:O	1:B:75:ASN:HB2	2.04	0.57
1:H:21:ILE:O	1:H:24:VAL:HG22	2.04	0.57
1:T:9:LEU:H	1:T:260:ASN:ND2	2.03	0.57
1:T:296:ASN:HD21	1:T:370:ASN:HD21	1.53	0.57
1:G:45:ARG:HA	1:G:52:VAL:HG21	1.86	0.57
1:K:276:LEU:HD12	1:K:357:MET:HE3	1.86	0.57
1:P:21:ILE:HD11	1:P:55:THR:HB	1.85	0.57
1:S:89:ARG:CD	1:S:89:ARG:NH1	2.67	0.57
1:M:265:TYR:H	1:M:370:ASN:ND2	2.03	0.57
1:B:266:VAL:HG12	1:B:285:ASN:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ALA:HB3	3:H:1441:HOH:O	2.03	0.57
1:P:180:ASP:HB3	1:P:183:LEU:HD22	1.87	0.56
1:F:4:ARG:N	3:F:1394:HOH:O	2.38	0.56
1:L:222:GLN:HE21	1:L:222:GLN:HA	1.70	0.56
1:P:153:HIS:HD2	1:P:168:VAL:HG22	1.70	0.56
1:R:9:LEU:HB3	1:R:173:LEU:HD21	1.87	0.56
1:A:265:TYR:H	1:A:370:ASN:HD22	1.52	0.56
1:A:277:TYR:HE2	1:A:357:MET:HE1	1.69	0.56
1:D:213:ASN:ND2	1:D:216:THR:H	2.03	0.56
1:E:266:VAL:HG12	1:E:285:ASN:HD22	1.69	0.56
1:J:152:ARG:H	1:J:259:ASN:ND2	2.02	0.56
1:M:233:GLN:HE21	1:M:233:GLN:N	1.95	0.56
1:N:27:ARG:HD3	3:N:1391:HOH:O	2.03	0.56
1:A:296:ASN:HD21	1:A:370:ASN:HD21	1.53	0.56
1:B:152:ARG:H	1:B:259:ASN:HD21	1.54	0.56
1:D:55:THR:O	1:D:59:LEU:HB2	2.05	0.56
1:S:89:ARG:CD	1:S:89:ARG:HH11	2.18	0.56
1:D:328:ILE:O	1:D:332:THR:HG22	2.06	0.56
1:I:9:LEU:H	1:I:260:ASN:HD21	1.52	0.56
1:O:230:ASN:OD1	1:O:246:TYR:HD2	1.88	0.56
1:A:277:TYR:CE2	1:A:357:MET:HE1	2.41	0.56
1:D:144:ALA:H	1:D:187:LYS:NZ	2.03	0.56
1:H:152:ARG:H	1:H:259:ASN:ND2	2.03	0.56
1:J:210:LYS:HE2	1:J:368:PHE:O	2.05	0.56
1:M:276:LEU:HD12	1:M:357:MET:HE3	1.88	0.56
1:I:152:ARG:NH1	1:I:259:ASN:O	2.38	0.56
1:C:222:GLN:HE21	1:C:222:GLN:HA	1.70	0.56
1:O:222:GLN:HE21	1:O:222:GLN:HA	1.71	0.56
1:S:233:GLN:HE21	1:S:233:GLN:N	2.03	0.56
1:L:213:ASN:HD22	1:L:215:VAL:H	1.51	0.55
1:R:152:ARG:H	1:R:259:ASN:ND2	2.01	0.55
1:E:280:PRO:HB2	1:E:283:VAL:HG13	1.87	0.55
1:F:152:ARG:HG3	1:F:168:VAL:HG13	1.88	0.55
1:J:187:LYS:HB2	1:J:244:ARG:HH22	1.71	0.55
1:L:142:THR:HG22	1:L:142:THR:O	2.04	0.55
1:N:375:ASN:C	1:N:375:ASN:HD22	2.13	0.55
1:C:55:THR:O	1:C:59:LEU:HB2	2.06	0.55
1:H:142:THR:O	1:H:142:THR:HG22	2.06	0.55
1:J:231:LEU:HD13	1:J:247:MET:HE2	1.88	0.55
1:T:265:TYR:H	1:T:370:ASN:ND2	2.04	0.55
1:B:233:GLN:HE21	1:B:233:GLN:N	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:VAL:HG22	1:H:292:VAL:HB	1.89	0.55
1:H:375:ASN:C	1:H:375:ASN:HD22	2.15	0.55
1:J:105:HIS:HE1	1:J:141:ASN:HD22	1.55	0.55
1:T:103:SER:HB2	1:T:104:PRO:HD3	1.89	0.55
1:N:265:TYR:H	1:N:370:ASN:ND2	2.05	0.55
1:P:105:HIS:HE1	1:P:141:ASN:HD22	1.55	0.55
1:J:98:THR:OG1	1:J:105:HIS:CD2	2.58	0.55
1:M:142:THR:O	1:M:142:THR:HG22	2.06	0.55
1:D:233:GLN:H	1:D:233:GLN:NE2	1.96	0.55
1:P:48:LYS:C	1:P:49:ASP:OD1	2.50	0.55
1:Q:216:THR:HG21	1:Q:261:ALA:HB2	1.89	0.55
1:Q:280:PRO:HB2	1:Q:283:VAL:HG12	1.89	0.55
1:A:216:THR:HG21	1:A:261:ALA:HB2	1.89	0.54
1:D:4:ARG:N	3:D:1435:HOH:O	2.40	0.54
1:F:200:LEU:O	1:F:204:VAL:HG13	2.07	0.54
1:O:13:VAL:HB	1:O:176:VAL:HG22	1.87	0.54
1:P:151:THR:CG2	1:P:153:HIS:H	2.20	0.54
1:E:296:ASN:HD21	1:E:370:ASN:HD21	1.53	0.54
1:K:265:TYR:H	1:K:370:ASN:ND2	2.05	0.54
1:S:382:ILE:HA	1:S:385:GLN:HE21	1.72	0.54
1:G:21:ILE:O	1:G:24:VAL:HG22	2.07	0.54
1:G:49:ASP:N	1:G:49:ASP:OD1	2.41	0.54
1:N:152:ARG:H	1:N:259:ASN:HD21	1.54	0.54
1:P:9:LEU:HB3	1:P:173:LEU:HD21	1.90	0.54
1:A:145:GLY:HA3	1:A:195:THR:O	2.07	0.54
1:I:151:THR:CG2	1:I:153:HIS:H	2.20	0.54
1:M:375:ASN:C	1:M:375:ASN:HD22	2.15	0.54
1:R:93:CYS:SG	1:R:93:CYS:CA	2.93	0.54
1:B:55:THR:HG21	1:B:99:VAL:HG11	1.90	0.54
1:K:188:PRO:O	1:K:192:THR:HG22	2.07	0.54
1:Q:233:GLN:H	1:Q:233:GLN:NE2	1.96	0.54
1:G:265:TYR:H	1:G:370:ASN:ND2	2.06	0.54
1:P:280:PRO:HB2	1:P:283:VAL:CG1	2.38	0.54
1:G:216:THR:HG21	1:G:261:ALA:CB	2.35	0.54
1:G:280:PRO:HB2	1:G:283:VAL:HG22	1.89	0.54
1:I:152:ARG:H	1:I:259:ASN:HD21	1.55	0.54
1:R:88:PHE:CD1	1:R:93:CYS:HB2	2.43	0.54
1:D:100:GLY:HA3	1:D:104:PRO:HG2	1.90	0.54
1:E:21:ILE:O	1:E:24:VAL:CG2	2.52	0.54
1:I:50:GLY:HA2	1:I:53:ASP:HB2	1.90	0.54
1:S:187:LYS:HE3	1:S:192:THR:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASP:OD2	1:B:152:ARG:NH2	2.36	0.54
1:E:265:TYR:H	1:E:370:ASN:ND2	2.06	0.54
1:K:50:GLY:HA3	3:K:1477:HOH:O	2.07	0.54
1:M:113:ILE:HD11	1:M:172:ASN:HD21	1.72	0.54
1:H:121:LEU:HD22	3:H:1410:HOH:O	2.08	0.53
1:J:20:ALA:O	1:J:23:VAL:HG22	2.07	0.53
1:K:210:LYS:HE2	1:K:368:PHE:O	2.09	0.53
1:S:265:TYR:H	1:S:370:ASN:ND2	2.06	0.53
1:N:125:ALA:HA	1:N:167:ILE:HG12	1.90	0.53
1:O:45:ARG:C	1:O:48:LYS:HB2	2.32	0.53
1:O:105:HIS:HE1	1:O:141:ASN:HD22	1.56	0.53
1:S:55:THR:O	1:S:59:LEU:HB2	2.08	0.53
1:G:52:VAL:HG12	1:G:99:VAL:CG2	2.38	0.53
1:P:9:LEU:HD22	1:Q:13:VAL:HG22	1.91	0.53
1:H:274:GLY:O	1:H:278:ASP:HA	2.08	0.53
1:C:180:ASP:HB3	1:C:183:LEU:HD22	1.90	0.53
1:D:151:THR:HG23	1:D:153:HIS:H	1.73	0.53
1:Q:24:VAL:HG13	1:Q:178:ILE:HD12	1.91	0.53
1:B:48:LYS:HB3	1:B:49:ASP:OD2	2.08	0.53
1:E:13:VAL:HG22	1:I:9:LEU:HD22	1.90	0.53
1:F:222:GLN:HE21	1:F:222:GLN:HA	1.73	0.53
1:H:216:THR:HG22	3:H:1429:HOH:O	2.07	0.53
1:J:128:GLU:OE2	1:J:169:SER:HA	2.08	0.53
1:L:109:LYS:NZ	1:L:151:THR:HG22	2.23	0.53
1:N:45:ARG:O	1:N:48:LYS:HE2	2.09	0.53
1:K:266:VAL:HG12	1:K:285:ASN:HD22	1.74	0.53
1:T:151:THR:HG22	1:T:153:HIS:N	2.22	0.53
1:B:173:LEU:HD23	1:O:12:ASN:OD1	2.09	0.53
1:H:121:LEU:CG	1:H:122:TYR:H	2.20	0.53
1:N:121:LEU:HG	1:N:122:TYR:H	1.72	0.53
1:A:173:LEU:HD23	1:D:12:ASN:OD1	2.09	0.53
1:E:119:GLY:O	1:E:120:ASP:HB2	2.09	0.53
1:G:213:ASN:C	1:G:213:ASN:HD22	2.17	0.53
1:M:119:GLY:O	1:M:120:ASP:CB	2.57	0.53
1:N:375:ASN:ND2	1:N:378:GLU:H	2.07	0.53
1:L:296:ASN:HD21	1:L:370:ASN:HD21	1.57	0.52
1:B:21:ILE:O	1:B:24:VAL:HG22	2.10	0.52
1:G:153:HIS:HD2	1:G:168:VAL:HG22	1.74	0.52
1:J:375:ASN:ND2	1:J:378:GLU:H	2.07	0.52
1:A:105:HIS:CE1	1:A:141:ASN:HD22	2.25	0.52
1:E:9:LEU:HB3	1:E:173:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:ASN:HD22	1:F:375:ASN:C	2.16	0.52
1:H:265:TYR:H	1:H:370:ASN:ND2	2.08	0.52
1:R:333:ARG:NH1	1:S:321:LEU:HB3	2.24	0.52
1:T:13:VAL:O	1:T:176:VAL:HA	2.09	0.52
1:A:98:THR:OG1	1:A:105:HIS:HD2	1.93	0.52
1:B:213:ASN:HD22	1:B:215:VAL:H	1.56	0.52
1:P:328:ILE:O	1:P:332:THR:HG23	2.09	0.52
1:C:16:PHE:HE1	1:F:8:TYR:HB2	1.74	0.52
1:G:296:ASN:HD21	1:G:370:ASN:HD21	1.57	0.52
1:O:128:GLU:OE2	1:O:169:SER:HA	2.09	0.52
1:C:45:ARG:O	1:C:48:LYS:N	2.42	0.52
1:C:105:HIS:HE1	1:C:141:ASN:HD22	1.57	0.52
1:E:74:PRO:O	1:E:75:ASN:HB2	2.10	0.52
1:G:231:LEU:O	1:G:235:VAL:HG13	2.09	0.52
1:K:231:LEU:O	1:K:235:VAL:HG13	2.09	0.52
1:M:49:ASP:OD1	1:M:49:ASP:N	2.42	0.52
1:A:265:TYR:H	1:A:370:ASN:ND2	2.08	0.52
1:H:222:GLN:HE21	1:H:222:GLN:HA	1.73	0.52
1:M:213:ASN:ND2	1:M:216:THR:H	2.08	0.52
1:S:49:ASP:OD1	1:S:49:ASP:N	2.42	0.52
1:A:171:ARG:CG	1:A:171:ARG:NH1	2.66	0.52
1:P:151:THR:HG23	1:P:153:HIS:H	1.74	0.52
1:P:273:LEU:HD23	1:P:357:MET:HE1	1.92	0.52
1:S:334:LEU:O	1:S:338:ILE:HG12	2.10	0.52
1:F:41:ASP:HB2	1:F:44:LEU:HD12	1.91	0.52
1:M:78:ASP:CB	1:M:121:LEU:HD13	2.40	0.52
1:N:181:PRO:HA	1:N:184:MET:HG3	1.92	0.52
1:G:265:TYR:H	1:G:370:ASN:HD22	1.57	0.52
1:O:200:LEU:HG	1:O:227:ILE:HG21	1.92	0.52
1:F:13:VAL:O	1:F:176:VAL:HA	2.11	0.51
1:T:280:PRO:HB2	1:T:283:VAL:HG22	1.91	0.51
1:M:82:ARG:HH11	1:M:121:LEU:HD21	1.74	0.51
1:N:266:VAL:HG12	1:N:285:ASN:HD22	1.74	0.51
1:A:266:VAL:HG12	1:A:285:ASN:HD22	1.75	0.51
1:I:328:ILE:O	1:I:332:THR:HG22	2.09	0.51
1:O:48:LYS:N	3:O:1407:HOH:O	2.43	0.51
1:Q:274:GLY:HA2	1:Q:278:ASP:HA	1.92	0.51
1:S:65:GLU:HB2	3:S:1394:HOH:O	2.09	0.51
1:A:24:VAL:HG22	1:A:178:ILE:CD1	2.41	0.51
1:B:152:ARG:HG3	1:B:168:VAL:HG13	1.92	0.51
1:I:222:GLN:HA	1:I:222:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:TYR:H	1:I:370:ASN:ND2	2.08	0.51
1:J:277:TYR:CE2	1:J:357:MET:HE1	2.46	0.51
1:J:296:ASN:HD21	1:J:370:ASN:HD21	1.58	0.51
1:N:119:GLY:O	1:N:120:ASP:HB2	2.10	0.51
1:Q:151:THR:CG2	1:Q:153:HIS:H	2.23	0.51
1:D:50:GLY:HA3	3:D:1391:HOH:O	2.11	0.51
1:T:45:ARG:C	1:T:48:LYS:HB2	2.34	0.51
1:G:344:LEU:HB2	1:G:387:PHE:HA	1.91	0.51
1:H:277:TYR:HE2	1:H:357:MET:HE1	1.76	0.51
1:S:16:PHE:HE1	1:T:8:TYR:HB2	1.76	0.51
1:T:263:LEU:HD13	1:T:267:HIS:CG	2.45	0.51
1:A:44:LEU:HD11	1:A:100:GLY:HA2	1.93	0.51
1:B:152:ARG:H	1:B:259:ASN:ND2	2.09	0.51
1:S:21:ILE:HD11	1:S:55:THR:HG22	1.92	0.51
1:K:4:ARG:NH2	3:K:1453:HOH:O	2.44	0.51
1:Q:60:ARG:HG3	1:Q:60:ARG:NH1	2.21	0.51
1:D:81:VAL:HG21	1:D:156:LEU:HD21	1.92	0.51
1:K:283:VAL:O	1:K:287:VAL:HG12	2.11	0.51
1:S:16:PHE:CE1	1:T:8:TYR:HB2	2.45	0.51
1:F:266:VAL:HG12	1:F:285:ASN:HD22	1.76	0.51
1:H:328:ILE:O	1:H:332:THR:HG22	2.11	0.51
1:K:280:PRO:HB2	1:K:283:VAL:HG13	1.93	0.51
1:T:9:LEU:H	1:T:260:ASN:HD21	1.59	0.51
1:L:213:ASN:ND2	1:L:216:THR:H	2.09	0.50
1:C:256:MET:HE3	3:C:1390:HOH:O	2.11	0.50
1:A:13:VAL:HB	1:A:176:VAL:HG22	1.92	0.50
1:B:230:ASN:OD1	1:B:246:TYR:HD2	1.93	0.50
1:D:144:ALA:H	1:D:187:LYS:HZ3	1.60	0.50
1:F:187:LYS:HB3	1:F:192:THR:HG22	1.93	0.50
1:H:216:THR:CG2	1:H:261:ALA:HB2	2.41	0.50
1:J:74:PRO:O	1:J:75:ASN:HB2	2.11	0.50
1:K:45:ARG:C	1:K:48:LYS:HB2	2.37	0.50
1:L:78:ASP:HB2	1:L:121:LEU:HD13	1.94	0.50
1:O:153:HIS:CD2	1:O:168:VAL:HG22	2.45	0.50
1:E:230:ASN:OD1	1:E:246:TYR:HD2	1.95	0.50
1:F:152:ARG:H	1:F:259:ASN:ND2	2.06	0.50
1:K:216:THR:HG23	3:K:1395:HOH:O	2.11	0.50
1:I:42:LYS:HG2	1:I:70:ASP:O	2.12	0.50
1:K:98:THR:OG1	1:K:105:HIS:HD2	1.94	0.50
1:S:296:ASN:HD21	1:S:370:ASN:HD21	1.58	0.50
1:H:187:LYS:HD2	1:H:191:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:216:THR:HG21	1:P:261:ALA:HB2	1.92	0.50
1:R:375:ASN:ND2	1:R:378:GLU:H	2.09	0.50
1:I:378:GLU:O	1:I:382:ILE:HG13	2.12	0.50
1:J:103:SER:HB2	1:J:104:PRO:HD3	1.93	0.50
1:K:227:ILE:HG12	1:K:247:MET:HE1	1.94	0.50
1:S:290:PRO:HB3	1:S:332:THR:HG22	1.93	0.50
1:A:222:GLN:HA	1:A:222:GLN:HE21	1.75	0.50
1:B:216:THR:HG21	1:B:261:ALA:HB2	1.93	0.50
1:M:116:THR:HG22	1:M:132:ASN:HB2	1.94	0.50
1:Q:21:ILE:HD11	1:Q:55:THR:HB	1.93	0.50
1:S:11:PRO:HD2	1:S:150:VAL:HG23	1.94	0.50
1:T:21:ILE:HD11	1:T:55:THR:HB	1.93	0.50
1:B:317:GLY:HA3	3:B:1401:HOH:O	2.11	0.50
1:H:142:THR:O	1:H:142:THR:CG2	2.60	0.50
1:H:151:THR:CG2	1:H:153:HIS:H	2.25	0.50
1:H:152:ARG:HH12	1:H:260:ASN:HD22	1.60	0.50
1:H:290:PRO:HG3	1:H:331:ILE:HG22	1.93	0.50
1:J:45:ARG:O	1:J:48:LYS:HB2	2.11	0.50
1:L:317:GLY:O	1:S:314:ASN:ND2	2.43	0.50
1:N:49:ASP:HB3	3:N:1415:HOH:O	2.12	0.50
1:D:152:ARG:HG3	1:D:168:VAL:HG13	1.93	0.49
1:J:50:GLY:HA2	1:J:53:ASP:HB2	1.94	0.49
1:K:119:GLY:O	1:K:120:ASP:HB2	2.12	0.49
1:C:265:TYR:H	1:C:370:ASN:ND2	2.10	0.49
1:H:180:ASP:HB3	1:H:183:LEU:HD22	1.93	0.49
1:M:266:VAL:HG12	1:M:285:ASN:HD22	1.77	0.49
1:N:52:VAL:O	1:N:56:LEU:HB2	2.12	0.49
1:E:82:ARG:HH22	1:E:121:LEU:CD2	2.24	0.49
1:H:230:ASN:OD1	1:H:246:TYR:HD2	1.94	0.49
1:M:21:ILE:HD11	1:M:55:THR:HB	1.94	0.49
1:P:152:ARG:H	1:P:259:ASN:ND2	2.09	0.49
1:I:82:ARG:NH1	1:I:121:LEU:HD21	2.27	0.49
1:H:188:PRO:O	1:H:192:THR:HG23	2.11	0.49
1:I:231:LEU:O	1:I:235:VAL:HG13	2.13	0.49
1:S:375:ASN:C	1:S:375:ASN:HD22	2.20	0.49
1:B:253:LEU:HD11	1:O:215:VAL:HA	1.94	0.49
1:C:266:VAL:HG12	1:C:285:ASN:HD22	1.77	0.49
1:F:307:ILE:O	1:F:311:MET:HG3	2.12	0.49
1:G:109:LYS:NZ	1:G:151:THR:HG22	2.28	0.49
1:I:45:ARG:HA	1:I:52:VAL:HG21	1.95	0.49
1:L:45:ARG:HA	1:L:52:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:375:ASN:C	1:O:375:ASN:HD22	2.21	0.49
1:P:40:THR:O	1:P:70:ASP:HA	2.12	0.49
1:A:151:THR:HG21	3:A:1404:HOH:O	2.13	0.49
1:C:103:SER:HB2	1:C:104:PRO:HD3	1.94	0.49
1:G:95:ILE:HG13	1:G:136:PRO:O	2.12	0.49
1:I:289:LEU:HB3	1:I:290:PRO:HD3	1.94	0.49
1:P:11:PRO:HB2	1:P:14:ASN:HD21	1.78	0.49
1:C:98:THR:HG21	1:C:108:GLY:HA3	1.94	0.49
1:J:344:LEU:HB2	1:J:387:PHE:HA	1.94	0.49
1:K:151:THR:CG2	1:K:153:HIS:H	2.25	0.49
1:P:100:GLY:HA3	1:P:104:PRO:HG2	1.94	0.49
1:F:45:ARG:HA	1:F:52:VAL:HG21	1.95	0.48
1:I:333:ARG:NH2	1:R:322:ASP:OD1	2.46	0.48
1:K:144:ALA:H	1:K:187:LYS:NZ	2.11	0.48
1:K:291:HIS:CD2	3:K:1447:HOH:O	2.58	0.48
1:S:9:LEU:H	1:S:260:ASN:HD21	1.60	0.48
1:T:200:LEU:HG	1:T:227:ILE:HG21	1.94	0.48
1:A:375:ASN:HD22	1:A:375:ASN:C	2.22	0.48
1:H:171:ARG:CG	1:H:171:ARG:NH1	2.64	0.48
1:K:50:GLY:HA2	1:K:53:ASP:HB2	1.95	0.48
1:L:55:THR:O	1:L:59:LEU:HB2	2.13	0.48
1:P:227:ILE:HG12	1:P:247:MET:HE1	1.94	0.48
1:S:50:GLY:HA3	3:S:1406:HOH:O	2.12	0.48
1:T:152:ARG:NH1	1:T:260:ASN:HD22	2.11	0.48
1:D:103:SER:HB2	1:D:104:PRO:HD3	1.95	0.48
1:I:375:ASN:ND2	1:I:378:GLU:H	2.12	0.48
1:P:113:ILE:HD11	1:P:172:ASN:HD21	1.79	0.48
1:R:203:ALA:HB1	1:R:224:ILE:HG13	1.95	0.48
1:S:151:THR:HG22	1:S:153:HIS:H	1.79	0.48
1:E:20:ALA:O	1:E:23:VAL:HG22	2.13	0.48
1:M:105:HIS:HE1	1:M:141:ASN:HD22	1.61	0.48
1:O:98:THR:OG1	1:O:105:HIS:HD2	1.95	0.48
1:A:280:PRO:HB2	1:A:283:VAL:HG22	1.94	0.48
1:B:273:LEU:HD23	1:B:357:MET:HE1	1.95	0.48
1:H:230:ASN:OD1	1:H:246:TYR:CD2	2.66	0.48
1:L:11:PRO:HD2	1:L:150:VAL:HG22	1.96	0.48
1:P:290:PRO:CB	1:P:332:THR:HG22	2.44	0.48
1:S:89:ARG:HH11	1:S:89:ARG:HD2	1.77	0.48
1:A:146:THR:HG23	1:A:148:SER:H	1.78	0.48
1:J:21:ILE:HD11	1:J:55:THR:HB	1.96	0.48
1:N:55:THR:O	1:N:59:LEU:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:98:THR:OG1	1:S:105:HIS:HD2	1.96	0.48
1:A:152:ARG:H	1:A:259:ASN:HD21	1.61	0.48
1:I:298:ILE:HD11	1:I:372:ARG:CZ	2.44	0.48
1:P:375:ASN:C	1:P:375:ASN:HD22	2.21	0.48
1:C:13:VAL:HG22	1:F:9:LEU:HD22	1.94	0.48
3:H:1408:HOH:O	1:I:325:GLU:HG2	2.13	0.48
1:K:180:ASP:HB3	1:K:183:LEU:HD22	1.96	0.48
1:K:213:ASN:H	1:K:216:THR:HG22	1.79	0.48
1:K:241:LEU:HD22	1:K:245:GLU:HG3	1.96	0.48
1:O:55:THR:O	1:O:59:LEU:HB2	2.14	0.48
1:R:188:PRO:O	1:R:192:THR:HG23	2.13	0.48
1:C:39:VAL:HB	1:C:98:THR:HG22	1.96	0.48
1:I:142:THR:HG22	1:I:142:THR:O	2.13	0.48
1:N:233:GLN:HE21	1:N:233:GLN:N	1.97	0.48
1:Q:231:LEU:O	1:Q:235:VAL:HG13	2.14	0.48
1:G:13:VAL:HG22	1:R:9:LEU:HD22	1.94	0.48
1:G:266:VAL:HG12	1:G:285:ASN:HD22	1.79	0.48
1:O:154:CYS:SG	1:O:156:LEU:HD21	2.54	0.48
1:R:41:ASP:HB2	1:R:44:LEU:HD12	1.96	0.48
1:D:283:VAL:O	1:D:287:VAL:HG12	2.13	0.47
1:G:277:TYR:CE2	1:G:357:MET:HE1	2.49	0.47
1:B:265:TYR:H	1:B:370:ASN:ND2	2.12	0.47
1:B:375:ASN:C	1:B:375:ASN:HD22	2.22	0.47
1:C:321:LEU:HD11	1:J:232:ARG:NH2	2.30	0.47
1:P:344:LEU:HB2	1:P:387:PHE:HA	1.95	0.47
1:R:38:LEU:HB3	1:R:68:ILE:HB	1.96	0.47
1:J:9:LEU:HB3	1:J:173:LEU:HD21	1.96	0.47
1:K:213:ASN:HD22	1:K:215:VAL:H	1.62	0.47
1:K:375:ASN:ND2	1:K:378:GLU:H	2.11	0.47
1:Q:152:ARG:H	1:Q:259:ASN:ND2	2.10	0.47
1:K:296:ASN:HD21	1:K:370:ASN:ND2	2.09	0.47
1:N:148:SER:HA	1:N:151:THR:HB	1.97	0.47
1:P:231:LEU:O	1:P:235:VAL:HG13	2.14	0.47
1:E:200:LEU:O	1:E:204:VAL:HG13	2.14	0.47
1:N:99:VAL:HB	1:N:140:VAL:HG13	1.97	0.47
1:T:222:GLN:HE21	1:T:222:GLN:HA	1.78	0.47
1:D:116:THR:HG21	1:D:133:PRO:O	2.15	0.47
1:F:38:LEU:HD11	1:F:99:VAL:CG1	2.44	0.47
1:G:277:TYR:HE2	1:G:357:MET:HE1	1.80	0.47
1:N:21:ILE:O	1:N:24:VAL:HG22	2.15	0.47
1:B:17:GLY:C	1:B:181:PRO:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLN:HA	1:B:222:GLN:HE21	1.80	0.47
1:C:9:LEU:HD22	1:F:13:VAL:HG22	1.96	0.47
1:C:213:ASN:ND2	1:C:216:THR:H	2.13	0.47
1:H:368:PHE:HB2	3:H:1399:HOH:O	2.14	0.47
1:I:216:THR:HG21	1:I:261:ALA:HB2	1.95	0.47
1:L:39:VAL:HB	1:L:98:THR:HG22	1.97	0.47
1:M:21:ILE:O	1:M:24:VAL:HG22	2.14	0.47
1:N:152:ARG:H	1:N:259:ASN:ND2	2.12	0.47
1:Q:41:ASP:HB2	1:Q:44:LEU:HD12	1.96	0.47
1:S:118:GLU:O	1:S:120:ASP:N	2.47	0.47
1:F:265:TYR:H	1:F:370:ASN:ND2	2.12	0.47
1:S:50:GLY:HA2	1:S:53:ASP:HB2	1.97	0.47
1:M:13:VAL:HB	1:M:176:VAL:HG22	1.96	0.47
1:M:213:ASN:HD22	1:M:215:VAL:H	1.62	0.47
1:O:171:ARG:HG2	1:O:171:ARG:NH1	2.24	0.47
1:S:222:GLN:HE21	1:S:222:GLN:HA	1.79	0.47
1:T:152:ARG:H	1:T:259:ASN:ND2	2.08	0.47
1:K:121:LEU:HA	3:K:1398:HOH:O	2.14	0.47
1:P:200:LEU:HG	1:P:227:ILE:HG21	1.95	0.47
1:C:216:THR:CG2	1:C:261:ALA:HB2	2.40	0.46
1:D:274:GLY:O	1:D:278:ASP:HA	2.14	0.46
1:I:151:THR:HG23	1:I:153:HIS:H	1.80	0.46
1:K:45:ARG:HA	1:K:52:VAL:HG21	1.97	0.46
1:L:18:PRO:HD2	1:M:4:ARG:O	2.15	0.46
1:N:39:VAL:HB	1:N:98:THR:HG22	1.97	0.46
1:R:210:LYS:HE2	1:R:368:PHE:O	2.14	0.46
1:T:21:ILE:O	1:T:24:VAL:HG22	2.15	0.46
1:B:5:MET:HG3	1:O:20:ALA:HA	1.96	0.46
1:B:13:VAL:HB	1:B:176:VAL:HG22	1.97	0.46
1:J:151:THR:HG23	1:J:153:HIS:H	1.79	0.46
1:K:265:TYR:H	1:K:370:ASN:HD22	1.61	0.46
1:P:266:VAL:HG12	1:P:285:ASN:HD22	1.80	0.46
1:B:45:ARG:HA	1:B:52:VAL:HG21	1.98	0.46
1:D:328:ILE:O	1:D:332:THR:CG2	2.63	0.46
1:H:27:ARG:HD3	3:H:1389:HOH:O	2.14	0.46
1:K:121:LEU:CG	1:K:122:TYR:H	2.28	0.46
1:O:103:SER:HB2	1:O:104:PRO:HD3	1.96	0.46
1:P:142:THR:O	1:P:142:THR:CG2	2.63	0.46
1:Q:49:ASP:N	1:Q:49:ASP:OD1	2.48	0.46
1:D:200:LEU:HG	1:D:227:ILE:HG21	1.97	0.46
1:P:99:VAL:HB	1:P:140:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:375:ASN:ND2	1:Q:378:GLU:H	2.13	0.46
1:C:152:ARG:H	1:C:259:ASN:ND2	2.13	0.46
1:L:10:VAL:HG23	1:L:11:PRO:HD2	1.97	0.46
1:M:180:ASP:HB3	1:M:183:LEU:HD22	1.97	0.46
1:S:266:VAL:HG12	1:S:285:ASN:HD22	1.81	0.46
1:C:11:PRO:HD2	1:C:150:VAL:HG22	1.97	0.46
1:H:263:LEU:HD13	1:H:267:HIS:CG	2.51	0.46
1:J:100:GLY:HA3	1:J:104:PRO:HG2	1.96	0.46
1:N:117:HIS:HB3	1:N:124:TYR:CZ	2.50	0.46
1:A:230:ASN:OD1	1:A:246:TYR:HD2	1.98	0.46
1:H:152:ARG:HD2	1:H:259:ASN:ND2	2.31	0.46
1:E:151:THR:CG2	1:E:153:HIS:H	2.24	0.46
1:G:375:ASN:ND2	1:G:378:GLU:H	2.14	0.46
1:T:216:THR:HG21	1:T:261:ALA:CB	2.34	0.46
1:A:151:THR:CG2	1:A:153:HIS:H	2.24	0.46
1:D:233:GLN:HE21	1:D:233:GLN:N	1.98	0.46
1:E:155:VAL:HB	1:E:166:VAL:HG22	1.98	0.46
1:F:294:ARG:NH1	3:F:1395:HOH:O	2.49	0.46
1:M:55:THR:O	1:M:59:LEU:HB2	2.15	0.46
1:N:14:ASN:ND2	1:N:177:SER:OG	2.42	0.46
1:R:375:ASN:HD22	1:R:375:ASN:C	2.23	0.46
1:B:231:LEU:HD13	1:B:247:MET:HE2	1.98	0.46
1:D:148:SER:C	1:D:150:VAL:H	2.24	0.46
1:E:213:ASN:ND2	1:E:216:THR:H	2.14	0.46
1:F:230:ASN:OD1	1:F:246:TYR:HD2	1.99	0.46
1:L:21:ILE:HD11	1:L:55:THR:HB	1.98	0.46
1:M:78:ASP:HB3	1:M:121:LEU:HD13	1.97	0.46
1:N:180:ASP:HB3	1:N:183:LEU:HD22	1.96	0.46
1:T:11:PRO:HB2	1:T:14:ASN:HD21	1.81	0.46
1:T:200:LEU:O	1:T:204:VAL:HG13	2.16	0.46
1:D:39:VAL:HB	1:D:98:THR:HG22	1.97	0.45
1:I:98:THR:HG21	1:I:108:GLY:HA3	1.98	0.45
1:I:105:HIS:HE1	1:I:141:ASN:ND2	2.13	0.45
1:O:151:THR:CG2	1:O:153:HIS:H	2.28	0.45
1:S:157:THR:HA	1:S:164:LYS:HA	1.98	0.45
1:D:296:ASN:HD21	1:D:370:ASN:HD21	1.64	0.45
1:L:127:ILE:O	1:L:129:THR:N	2.49	0.45
1:N:278:ASP:CG	1:N:278:ASP:O	2.59	0.45
1:G:200:LEU:HG	1:G:227:ILE:HG21	1.99	0.45
1:H:273:LEU:HD23	1:H:357:MET:HE1	1.97	0.45
1:H:296:ASN:HD21	1:H:370:ASN:ND2	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:ILE:O	1:I:332:THR:CG2	2.65	0.45
1:K:152:ARG:HG3	1:K:168:VAL:HG13	1.97	0.45
1:K:274:GLY:O	1:K:278:ASP:HA	2.17	0.45
1:L:116:THR:HG21	1:L:133:PRO:O	2.16	0.45
1:S:216:THR:HG21	1:S:261:ALA:HB2	1.98	0.45
1:A:344:LEU:HD22	1:A:349:VAL:HG21	1.99	0.45
1:D:203:ALA:HB1	1:D:224:ILE:HG13	1.97	0.45
1:H:375:ASN:HD22	1:H:378:GLU:H	1.65	0.45
1:I:246:TYR:HE1	3:I:1420:HOH:O	1.99	0.45
1:J:216:THR:HG22	3:J:1406:HOH:O	2.16	0.45
1:L:77:LYS:HD3	1:L:157:THR:HB	1.99	0.45
1:P:152:ARG:HG3	1:P:168:VAL:HG13	1.97	0.45
1:P:180:ASP:OD2	1:P:182:LEU:HB2	2.16	0.45
1:A:121:LEU:HD22	3:A:1409:HOH:O	2.15	0.45
1:A:227:ILE:HG13	1:A:250:ALA:HB1	1.99	0.45
1:E:153:HIS:HD2	1:E:168:VAL:HG22	1.80	0.45
1:E:213:ASN:HD22	1:E:215:VAL:H	1.63	0.45
1:L:328:ILE:O	1:L:332:THR:HG22	2.16	0.45
1:P:213:ASN:HD22	1:P:215:VAL:H	1.65	0.45
1:R:277:TYR:CZ	1:R:349:VAL:HA	2.51	0.45
1:S:117:HIS:CB	3:S:1390:HOH:O	2.54	0.45
1:T:328:ILE:O	1:T:332:THR:CG2	2.64	0.45
1:B:280:PRO:HB2	1:B:283:VAL:HG13	1.99	0.45
1:F:119:GLY:O	1:F:120:ASP:HB2	2.16	0.45
1:J:45:ARG:C	1:J:48:LYS:N	2.75	0.45
1:R:180:ASP:HB3	1:R:183:LEU:HD22	1.99	0.45
1:B:51:ALA:HB3	3:B:1402:HOH:O	2.16	0.45
1:K:11:PRO:HD2	1:K:150:VAL:HG22	1.99	0.45
1:K:113:ILE:HA	1:K:134:LEU:HD22	1.98	0.45
1:Q:119:GLY:O	1:Q:120:ASP:HB2	2.17	0.45
1:T:10:VAL:HG21	1:T:256:MET:HE3	1.99	0.45
1:F:78:ASP:HB2	1:F:121:LEU:HD13	1.98	0.45
1:F:88:PHE:CD1	1:F:93:CYS:HB2	2.52	0.45
1:G:222:GLN:HE21	1:G:222:GLN:HA	1.81	0.45
1:H:49:ASP:OD1	1:H:49:ASP:N	2.49	0.45
1:H:78:ASP:OD1	1:H:78:ASP:N	2.48	0.45
1:J:82:ARG:NH1	1:J:121:LEU:HD21	2.32	0.45
1:M:37:LEU:HD22	1:M:88:PHE:HB2	1.98	0.45
1:O:276:LEU:HD12	1:O:357:MET:HE3	1.97	0.45
1:P:20:ALA:O	1:P:23:VAL:HG22	2.16	0.45
1:T:147:ALA:HB1	1:T:255:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HB3	1:L:352:THR:HB	1.99	0.45
1:C:16:PHE:CE1	1:F:8:TYR:HB2	2.52	0.45
1:I:20:ALA:O	1:I:23:VAL:HG22	2.17	0.45
1:L:95:ILE:HG13	1:L:136:PRO:O	2.17	0.45
1:P:48:LYS:O	1:P:49:ASP:OD1	2.35	0.45
1:T:11:PRO:HG3	1:T:174:PRO:HD2	1.99	0.45
1:E:315:ILE:HD13	1:E:315:ILE:HA	1.79	0.45
1:H:289:LEU:HB3	1:H:290:PRO:HD3	1.99	0.45
1:N:105:HIS:CE1	1:N:141:ASN:HD22	2.26	0.45
1:C:375:ASN:C	1:C:375:ASN:HD22	2.26	0.44
1:I:276:LEU:HD12	1:I:357:MET:HE3	1.99	0.44
1:B:188:PRO:O	1:B:192:THR:HG23	2.17	0.44
1:C:10:VAL:HG11	1:F:10:VAL:HG11	1.99	0.44
1:D:344:LEU:HB2	1:D:387:PHE:HA	1.98	0.44
1:I:204:VAL:O	1:I:208:ILE:HG12	2.17	0.44
1:L:134:LEU:HB3	1:L:135:PRO:HD2	1.99	0.44
1:N:266:VAL:HG22	1:N:292:VAL:HB	1.99	0.44
1:O:152:ARG:NH1	1:O:259:ASN:O	2.46	0.44
1:R:100:GLY:HA3	1:R:104:PRO:HG2	1.98	0.44
1:A:121:LEU:CG	1:A:122:TYR:H	2.31	0.44
1:C:273:LEU:HD23	1:C:357:MET:HE1	1.99	0.44
1:F:187:LYS:HB2	1:F:244:ARG:HH22	1.82	0.44
1:H:95:ILE:HG13	1:H:136:PRO:O	2.16	0.44
1:N:142:THR:HG23	1:N:183:LEU:HB3	1.99	0.44
1:S:375:ASN:ND2	1:S:378:GLU:H	2.16	0.44
1:T:216:THR:CG2	1:T:261:ALA:HB2	2.34	0.44
1:C:26:GLU:HA	1:C:29:GLN:HE21	1.82	0.44
1:D:109:LYS:NZ	1:D:151:THR:HG22	2.32	0.44
1:G:328:ILE:O	1:G:332:THR:CG2	2.65	0.44
1:I:103:SER:HB2	1:I:104:PRO:HD3	1.98	0.44
1:P:98:THR:OG1	1:P:105:HIS:HD2	1.99	0.44
1:Q:290:PRO:HG3	1:Q:331:ILE:HG22	1.98	0.44
1:R:142:THR:O	1:R:142:THR:HG22	2.17	0.44
1:B:226:LEU:HD22	1:B:246:TYR:HB3	1.99	0.44
1:D:216:THR:CG2	3:D:1429:HOH:O	2.45	0.44
1:K:142:THR:HG22	1:K:142:THR:O	2.18	0.44
1:K:272:GLN:C	1:K:357:MET:HE2	2.43	0.44
1:P:216:THR:HG22	1:P:217:ASP:N	2.33	0.44
1:S:85:LEU:HD13	1:S:115:ALA:HB2	1.98	0.44
1:A:74:PRO:O	1:A:75:ASN:HB2	2.16	0.44
1:A:210:LYS:HE2	1:A:368:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:MET:HA	1:A:360:MET:HE2	1.99	0.44
1:C:280:PRO:HB2	1:C:283:VAL:HG22	2.00	0.44
1:F:11:PRO:HD2	1:F:150:VAL:HG22	1.99	0.44
1:F:21:ILE:HD11	1:F:55:THR:HB	1.99	0.44
1:G:216:THR:CG2	1:G:261:ALA:HB2	2.40	0.44
1:K:119:GLY:O	1:K:120:ASP:CB	2.65	0.44
1:M:216:THR:HG22	1:M:217:ASP:N	2.33	0.44
1:S:328:ILE:O	1:S:332:THR:HG23	2.18	0.44
1:A:18:PRO:HG2	1:D:4:ARG:HG3	1.99	0.44
1:C:96:ILE:HB	1:C:137:ILE:HG12	2.00	0.44
1:E:9:LEU:HD22	1:I:13:VAL:HG22	1.99	0.44
1:H:103:SER:HB2	1:H:104:PRO:HD3	2.00	0.44
1:O:74:PRO:O	1:O:75:ASN:HB2	2.18	0.44
1:P:95:ILE:HG13	1:P:136:PRO:O	2.18	0.44
1:P:127:ILE:O	1:P:129:THR:N	2.50	0.44
1:B:325:GLU:HG2	3:Q:1401:HOH:O	2.18	0.44
1:C:142:THR:O	1:C:142:THR:HG22	2.18	0.44
1:H:74:PRO:O	1:H:75:ASN:HB2	2.16	0.44
1:L:283:VAL:O	1:L:287:VAL:HG12	2.17	0.44
1:L:375:ASN:ND2	1:L:378:GLU:H	2.15	0.44
1:O:127:ILE:H	1:O:127:ILE:HG13	1.63	0.44
1:O:231:LEU:O	1:O:235:VAL:HG13	2.18	0.44
1:A:242:GLN:HG2	1:A:246:TYR:CE2	2.52	0.44
1:B:153:HIS:HD2	1:B:168:VAL:HG22	1.83	0.44
1:H:77:LYS:O	1:H:80:ASN:HB2	2.17	0.44
1:M:242:GLN:HE21	1:M:246:TYR:HE2	1.65	0.44
1:S:18:PRO:HG2	1:T:4:ARG:HB2	1.99	0.44
1:S:35:LYS:HG2	3:S:1396:HOH:O	2.17	0.44
1:T:68:ILE:H	1:T:68:ILE:HG13	1.64	0.44
1:B:231:LEU:O	1:B:235:VAL:HG13	2.17	0.43
1:J:13:VAL:HG22	1:N:9:LEU:HD22	2.00	0.43
1:M:231:LEU:O	1:M:235:VAL:HG13	2.18	0.43
1:O:45:ARG:O	1:O:48:LYS:HB2	2.18	0.43
1:Q:263:LEU:HD13	1:Q:267:HIS:CG	2.53	0.43
1:S:117:HIS:O	1:S:118:GLU:C	2.61	0.43
1:A:144:ALA:H	1:A:187:LYS:NZ	2.16	0.43
1:E:233:GLN:HE21	1:E:233:GLN:N	1.99	0.43
1:F:121:LEU:HG	1:F:122:TYR:N	2.27	0.43
1:J:213:ASN:HD22	1:J:215:VAL:H	1.66	0.43
1:N:263:LEU:HD13	1:N:267:HIS:CG	2.53	0.43
1:S:152:ARG:CD	1:S:259:ASN:HD21	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:GLY:O	1:B:120:ASP:CB	2.61	0.43
1:C:8:TYR:HB2	1:F:16:PHE:HE1	1.82	0.43
1:I:98:THR:OG1	1:I:105:HIS:HD2	2.01	0.43
1:L:29:GLN:HG3	1:L:64:ILE:HD11	2.00	0.43
1:L:113:ILE:HA	1:L:134:LEU:HD22	2.00	0.43
1:Q:103:SER:HB2	1:Q:104:PRO:HD3	2.00	0.43
1:R:294:ARG:NH2	1:R:325:GLU:OE2	2.51	0.43
1:T:76:PRO:HB2	1:T:156:LEU:HD12	2.00	0.43
1:B:121:LEU:H	1:B:121:LEU:HG	1.53	0.43
1:E:180:ASP:HA	1:E:181:PRO:HD2	1.81	0.43
1:G:99:VAL:HG12	1:G:140:VAL:HG13	2.00	0.43
1:I:7:ASP:OD2	1:I:152:ARG:NH2	2.52	0.43
1:M:280:PRO:HB2	1:M:283:VAL:HG13	1.99	0.43
1:N:151:THR:CG2	1:N:153:HIS:H	2.24	0.43
1:O:328:ILE:O	1:O:332:THR:CG2	2.63	0.43
1:C:188:PRO:O	1:C:192:THR:HG23	2.18	0.43
1:M:152:ARG:NH1	1:M:260:ASN:HD22	2.16	0.43
1:N:77:LYS:HD3	1:N:157:THR:HB	1.98	0.43
1:Q:185:ILE:HD13	1:Q:244:ARG:HG2	2.00	0.43
1:A:51:ALA:HB3	3:A:1402:HOH:O	2.19	0.43
1:F:105:HIS:CD2	1:F:139:ALA:HB1	2.53	0.43
1:K:41:ASP:O	1:K:45:ARG:HB3	2.19	0.43
1:P:290:PRO:HG2	3:P:1408:HOH:O	2.19	0.43
1:R:204:VAL:O	1:R:208:ILE:HG12	2.18	0.43
1:E:95:ILE:HG13	1:E:136:PRO:O	2.19	0.43
1:G:127:ILE:H	1:G:127:ILE:HG13	1.68	0.43
1:G:204:VAL:O	1:G:208:ILE:HG12	2.19	0.43
1:H:283:VAL:O	1:H:287:VAL:HG12	2.19	0.43
1:H:322:ASP:OD1	1:L:333:ARG:NH2	2.52	0.43
1:N:213:ASN:C	1:N:213:ASN:HD22	2.26	0.43
1:R:144:ALA:H	1:R:187:LYS:NZ	2.16	0.43
1:E:360:MET:HE2	1:E:360:MET:HA	2.00	0.43
1:G:338:ILE:HG13	1:G:340:ILE:HG12	2.01	0.43
1:H:52:VAL:HG12	1:H:99:VAL:CG2	2.48	0.43
1:K:52:VAL:O	1:K:56:LEU:HB2	2.19	0.43
1:L:98:THR:OG1	1:L:105:HIS:HD2	2.02	0.43
1:N:121:LEU:HB2	1:N:165:PHE:CZ	2.53	0.43
1:S:38:LEU:HB3	1:S:68:ILE:HA	2.01	0.43
1:F:31:LEU:HD13	1:F:136:PRO:HB3	2.01	0.43
1:G:74:PRO:O	1:G:75:ASN:HB2	2.19	0.43
1:I:265:TYR:H	1:I:370:ASN:HD22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:274:GLY:O	1:I:278:ASP:HA	2.18	0.43
1:S:98:THR:HG21	1:S:108:GLY:HA3	2.01	0.43
1:S:354:PHE:N	1:S:355:PRO:HD2	2.34	0.43
1:A:152:ARG:H	1:A:259:ASN:ND2	2.16	0.43
1:A:180:ASP:HA	1:A:181:PRO:HD2	1.95	0.43
1:B:76:PRO:HB2	1:B:156:LEU:HD12	2.01	0.43
1:H:203:ALA:HB1	1:H:224:ILE:HG13	2.01	0.43
1:B:17:GLY:O	1:B:181:PRO:HD2	2.19	0.42
1:C:184:MET:O	1:C:187:LYS:HG3	2.19	0.42
1:H:113:ILE:HD11	1:H:172:ASN:HD21	1.83	0.42
1:H:227:ILE:HG13	1:H:250:ALA:HB1	2.00	0.42
1:I:121:LEU:HD23	3:I:1406:HOH:O	2.19	0.42
1:I:294:ARG:NH1	3:I:1436:HOH:O	2.43	0.42
1:L:7:ASP:CG	1:L:152:ARG:HH22	2.27	0.42
1:N:21:ILE:HD11	1:N:55:THR:HB	2.01	0.42
1:O:144:ALA:H	1:O:187:LYS:NZ	2.17	0.42
1:B:375:ASN:HD22	1:B:378:GLU:H	1.66	0.42
1:C:153:HIS:HD2	1:C:168:VAL:HG22	1.82	0.42
1:C:334:LEU:O	1:C:338:ILE:HG12	2.19	0.42
1:D:98:THR:HG21	1:D:108:GLY:HA3	2.01	0.42
1:F:103:SER:HB2	1:F:104:PRO:HD3	2.00	0.42
1:I:171:ARG:HG2	1:I:171:ARG:NH1	2.22	0.42
1:L:265:TYR:H	1:L:370:ASN:ND2	2.17	0.42
1:P:150:VAL:HG13	1:P:150:VAL:O	2.18	0.42
1:Q:9:LEU:HB3	1:Q:173:LEU:HD21	2.01	0.42
1:Q:181:PRO:HA	1:Q:184:MET:HG3	2.01	0.42
1:S:152:ARG:HD2	1:S:259:ASN:HD21	1.83	0.42
1:B:37:LEU:HD22	1:B:88:PHE:HB2	2.01	0.42
1:C:77:LYS:HD3	1:C:157:THR:HB	2.01	0.42
1:F:242:GLN:HG2	1:F:246:TYR:CE2	2.55	0.42
1:G:256:MET:HE1	1:R:8:TYR:CE2	2.54	0.42
1:H:222:GLN:HE22	1:H:225:ARG:HE	1.66	0.42
1:K:134:LEU:HD11	1:K:172:ASN:HD22	1.84	0.42
1:L:142:THR:O	1:L:142:THR:CG2	2.68	0.42
1:N:109:LYS:NZ	1:N:151:THR:HG22	2.35	0.42
1:R:85:LEU:HD22	1:R:114:ALA:HB1	2.00	0.42
1:R:221:MET:HG2	1:R:310:LEU:HD21	2.01	0.42
1:S:37:LEU:HD22	1:S:88:PHE:HD1	1.84	0.42
1:S:253:LEU:HD11	1:T:215:VAL:HA	2.00	0.42
1:B:105:HIS:HE1	1:B:141:ASN:HD22	1.67	0.42
1:B:152:ARG:HD2	1:B:259:ASN:ND2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:HG	1:C:227:ILE:HG21	1.99	0.42
1:G:39:VAL:HB	1:G:98:THR:HG22	2.01	0.42
1:H:375:ASN:ND2	1:H:378:GLU:H	2.17	0.42
1:L:152:ARG:HG3	1:L:168:VAL:HG13	2.02	0.42
1:A:95:ILE:HG13	1:A:136:PRO:O	2.18	0.42
1:I:152:ARG:HH12	1:I:260:ASN:HD22	1.66	0.42
1:J:127:ILE:H	1:J:127:ILE:HG13	1.67	0.42
1:M:95:ILE:HG13	1:M:136:PRO:O	2.19	0.42
1:M:121:LEU:HG	1:M:122:TYR:H	1.84	0.42
1:M:233:GLN:NE2	1:M:233:GLN:N	2.63	0.42
1:R:184:MET:HB3	1:R:187:LYS:HE2	2.01	0.42
1:S:152:ARG:H	1:S:259:ASN:HD21	1.67	0.42
1:T:187:LYS:HB2	1:T:244:ARG:HH22	1.83	0.42
1:A:145:GLY:HA2	1:A:199:ALA:HB2	2.01	0.42
1:I:21:ILE:HD11	1:I:55:THR:HG22	2.01	0.42
1:M:375:ASN:ND2	1:M:378:GLU:H	2.18	0.42
1:P:221:MET:HG2	1:P:310:LEU:HD21	2.02	0.42
1:Q:87:VAL:HG22	1:Q:90:ARG:HH22	1.84	0.42
1:Q:100:GLY:HA3	1:Q:104:PRO:HG2	2.01	0.42
1:R:76:PRO:HG3	1:R:103:SER:HA	2.02	0.42
1:S:39:VAL:HB	1:S:98:THR:HG22	2.02	0.42
1:A:375:ASN:ND2	1:A:378:GLU:H	2.17	0.42
1:M:222:GLN:HE21	1:M:222:GLN:HA	1.85	0.42
1:P:50:GLY:HA2	1:P:53:ASP:HB2	2.01	0.42
1:T:36:ALA:HA	1:T:95:ILE:O	2.20	0.42
1:T:181:PRO:HA	1:T:184:MET:HG3	2.02	0.42
1:E:82:ARG:HH22	1:E:121:LEU:HD21	1.83	0.42
1:F:82:ARG:NH2	1:F:121:LEU:HB3	2.34	0.42
1:K:121:LEU:HG	1:K:122:TYR:H	1.83	0.42
1:P:375:ASN:ND2	1:P:378:GLU:H	2.17	0.42
1:R:113:ILE:HG12	1:R:130:LEU:HD21	2.02	0.42
1:S:45:ARG:HA	1:S:52:VAL:HG21	2.01	0.42
1:S:203:ALA:HB1	1:S:224:ILE:HG13	2.02	0.42
1:J:203:ALA:HB1	1:J:224:ILE:HG13	2.02	0.42
1:K:127:ILE:H	1:K:127:ILE:HG13	1.67	0.42
1:P:120:ASP:OD2	1:P:121:LEU:HG	2.20	0.42
1:Q:13:VAL:O	1:Q:176:VAL:HA	2.20	0.42
1:I:216:THR:HG22	1:I:217:ASP:N	2.34	0.42
1:L:232:ARG:NH1	1:L:337:ASP:OD2	2.43	0.42
1:Q:98:THR:OG1	1:Q:105:HIS:HD2	2.03	0.42
1:Q:375:ASN:C	1:Q:375:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:13:VAL:HB	1:T:176:VAL:HG22	2.01	0.42
1:T:113:ILE:HA	1:T:134:LEU:HD22	2.02	0.42
1:B:375:ASN:ND2	1:B:378:GLU:H	2.18	0.41
1:C:187:LYS:HB2	1:C:244:ARG:HH22	1.85	0.41
1:H:233:GLN:NE2	1:H:233:GLN:N	2.53	0.41
1:J:127:ILE:O	1:J:129:THR:N	2.53	0.41
1:N:231:LEU:HD13	1:N:247:MET:HE2	2.02	0.41
1:R:294:ARG:HH11	1:R:328:ILE:HG21	1.85	0.41
1:A:121:LEU:HG	1:A:122:TYR:H	1.85	0.41
1:G:205:GLU:OE2	1:G:266:VAL:HG23	2.20	0.41
1:H:75:ASN:HD22	1:H:75:ASN:HA	1.65	0.41
1:H:151:THR:HG23	1:H:153:HIS:ND1	2.34	0.41
1:I:113:ILE:HA	1:I:134:LEU:HD22	2.01	0.41
1:M:227:ILE:HG12	1:M:247:MET:HE1	2.03	0.41
1:M:334:LEU:O	1:M:338:ILE:HG12	2.20	0.41
1:Q:45:ARG:O	1:Q:48:LYS:HE2	2.19	0.41
1:R:233:GLN:H	1:R:233:GLN:NE2	2.09	0.41
1:S:280:PRO:O	1:S:281:HIS:C	2.62	0.41
1:F:272:GLN:O	1:F:357:MET:HE2	2.20	0.41
1:H:48:LYS:C	1:H:49:ASP:OD1	2.63	0.41
1:Q:204:VAL:O	1:Q:208:ILE:HG12	2.20	0.41
1:S:95:ILE:HG13	1:S:136:PRO:O	2.21	0.41
1:B:23:VAL:O	1:B:24:VAL:C	2.64	0.41
1:B:266:VAL:HG22	1:B:292:VAL:HB	2.03	0.41
1:E:289:LEU:HD13	1:E:331:ILE:HG21	2.02	0.41
1:G:41:ASP:HB2	1:G:44:LEU:HD12	2.02	0.41
1:O:11:PRO:HD2	1:O:150:VAL:HG22	2.02	0.41
1:O:360:MET:HE2	1:O:360:MET:HA	2.01	0.41
1:P:74:PRO:O	1:P:75:ASN:HB2	2.21	0.41
1:P:127:ILE:HB	1:P:128:GLU:H	1.63	0.41
1:P:210:LYS:HE2	1:P:368:PHE:O	2.20	0.41
1:S:350:LYS:HB2	3:S:1397:HOH:O	2.20	0.41
1:A:24:VAL:HG22	1:A:178:ILE:HD12	2.01	0.41
1:E:52:VAL:HG13	3:E:1396:HOH:O	2.19	0.41
1:G:334:LEU:O	1:G:338:ILE:HG12	2.21	0.41
1:H:222:GLN:NE2	1:H:225:ARG:HE	2.18	0.41
1:H:334:LEU:O	1:H:338:ILE:HG12	2.19	0.41
1:K:116:THR:HG21	1:K:133:PRO:O	2.20	0.41
1:L:221:MET:HG2	1:L:310:LEU:HD21	2.03	0.41
1:F:210:LYS:HE2	1:F:368:PHE:O	2.20	0.41
1:H:99:VAL:HB	1:H:140:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ARG:NH1	1:H:259:ASN:O	2.54	0.41
1:K:375:ASN:C	1:K:375:ASN:ND2	2.78	0.41
1:N:48:LYS:HB3	1:N:49:ASP:H	1.65	0.41
1:P:6:PHE:HB2	1:Q:16:PHE:CE2	2.55	0.41
1:P:184:MET:O	1:P:187:LYS:HG3	2.20	0.41
1:R:88:PHE:CD1	1:R:93:CYS:CB	3.03	0.41
1:D:145:GLY:HA2	1:D:199:ALA:HB2	2.03	0.41
1:I:151:THR:HG22	1:I:153:HIS:H	1.85	0.41
1:N:216:THR:HG21	1:N:261:ALA:HB2	2.03	0.41
1:O:24:VAL:HG13	1:O:178:ILE:HD13	2.01	0.41
1:S:127:ILE:HB	1:S:128:GLU:H	1.62	0.41
1:T:144:ALA:HB3	1:T:187:LYS:HZ3	1.85	0.41
1:D:227:ILE:HG12	1:D:247:MET:HE1	2.02	0.41
1:E:216:THR:HG22	1:E:217:ASP:N	2.35	0.41
1:H:113:ILE:HG12	1:H:130:LEU:HD21	2.02	0.41
1:P:10:VAL:HG11	1:Q:10:VAL:HG11	2.02	0.41
1:P:11:PRO:HD2	1:P:150:VAL:HG22	2.02	0.41
1:T:15:PHE:O	1:T:178:ILE:HA	2.21	0.41
1:B:213:ASN:HB2	1:B:214:PRO:HD2	2.03	0.41
1:J:7:ASP:HB3	1:N:15:PHE:CE2	2.55	0.41
1:K:302:GLU:HG3	1:K:320:THR:HG21	2.02	0.41
1:L:103:SER:CB	1:L:104:PRO:HD3	2.47	0.41
1:L:375:ASN:HD22	1:L:378:GLU:H	1.69	0.41
1:M:298:ILE:HD11	1:M:372:ARG:CZ	2.50	0.41
1:N:200:LEU:O	1:N:204:VAL:HG13	2.21	0.41
1:Q:11:PRO:HD2	1:Q:150:VAL:HG22	2.02	0.41
1:S:152:ARG:H	1:S:259:ASN:ND2	2.19	0.41
1:T:127:ILE:HB	1:T:128:GLU:H	1.67	0.41
1:T:188:PRO:O	1:T:192:THR:HG22	2.21	0.41
1:T:264:GLY:HA3	1:T:370:ASN:HD22	1.86	0.41
1:A:75:ASN:HD22	1:A:75:ASN:HA	1.70	0.41
1:B:77:LYS:O	1:B:80:ASN:HB2	2.21	0.41
1:G:382:ILE:HA	1:G:385:GLN:HE21	1.86	0.41
1:H:11:PRO:HD2	1:H:150:VAL:HG22	2.03	0.41
1:H:204:VAL:O	1:H:208:ILE:HG12	2.21	0.41
1:M:13:VAL:O	1:M:176:VAL:HA	2.21	0.41
1:N:117:HIS:O	1:N:118:GLU:C	2.63	0.41
1:R:265:TYR:H	1:R:370:ASN:HD22	1.68	0.41
1:T:121:LEU:HD23	1:T:121:LEU:H	1.86	0.41
1:B:12:ASN:OD1	1:O:173:LEU:HD23	2.21	0.40
1:D:21:ILE:HD11	1:D:55:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ILE:O	1:F:24:VAL:HG22	2.21	0.40
1:K:95:ILE:HG13	1:K:136:PRO:O	2.20	0.40
1:K:127:ILE:O	1:K:129:THR:N	2.53	0.40
1:L:21:ILE:O	1:L:24:VAL:HG22	2.21	0.40
1:N:49:ASP:OD1	1:N:49:ASP:N	2.41	0.40
1:O:21:ILE:HD11	1:O:55:THR:HB	2.03	0.40
1:Q:184:MET:O	1:Q:187:LYS:HG3	2.21	0.40
1:S:280:PRO:O	1:S:282:GLY:N	2.55	0.40
1:T:298:ILE:HG23	3:T:1411:HOH:O	2.20	0.40
1:C:7:ASP:OD2	1:C:152:ARG:NH2	2.52	0.40
1:E:40:THR:O	1:E:70:ASP:HA	2.21	0.40
1:E:152:ARG:N	1:E:259:ASN:HD21	2.12	0.40
1:G:9:LEU:HB3	1:G:173:LEU:HD21	2.04	0.40
1:M:117:HIS:O	1:M:119:GLY:N	2.44	0.40
1:A:103:SER:HB2	1:A:104:PRO:HD3	2.03	0.40
1:C:277:TYR:HE2	1:C:357:MET:HE1	1.86	0.40
1:E:354:PHE:HB2	1:E:355:PRO:HD3	2.03	0.40
1:G:113:ILE:HG12	1:G:130:LEU:HD21	2.03	0.40
1:I:263:LEU:HD13	1:I:267:HIS:CG	2.57	0.40
1:Q:20:ALA:HB3	1:Q:180:ASP:HB2	2.03	0.40
1:B:150:VAL:O	1:B:150:VAL:HG13	2.21	0.40
1:B:334:LEU:O	1:B:338:ILE:HG12	2.22	0.40
1:C:152:ARG:HG3	1:C:168:VAL:HG13	2.03	0.40
1:H:232:ARG:NH2	1:I:321:LEU:HD11	2.35	0.40
1:J:152:ARG:HG3	1:J:168:VAL:HG13	2.03	0.40
1:O:13:VAL:O	1:O:176:VAL:HA	2.21	0.40
1:P:382:ILE:HA	1:P:385:GLN:HE21	1.86	0.40
1:A:127:ILE:HD12	1:A:128:GLU:H	1.85	0.40
1:D:60:ARG:NE	3:D:1413:HOH:O	2.54	0.40
1:G:121:LEU:H	1:G:121:LEU:CD2	2.30	0.40
1:G:152:ARG:NH1	1:G:259:ASN:O	2.55	0.40
1:H:119:GLY:O	1:H:120:ASP:CB	2.69	0.40
1:H:152:ARG:HH12	1:H:260:ASN:ND2	2.19	0.40
1:J:213:ASN:HD22	1:J:215:VAL:N	2.19	0.40
1:K:74:PRO:O	1:K:75:ASN:HB2	2.21	0.40
1:L:68:ILE:H	1:L:68:ILE:HG13	1.60	0.40
1:L:338:ILE:HG13	1:L:340:ILE:HG12	2.02	0.40
1:R:152:ARG:NH1	1:R:259:ASN:O	2.50	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	378/387 (98%)	361 (96%)	10 (3%)	7 (2%)	6	17
1	B	378/387 (98%)	356 (94%)	15 (4%)	7 (2%)	6	17
1	C	378/387 (98%)	357 (94%)	15 (4%)	6 (2%)	7	20
1	D	378/387 (98%)	357 (94%)	15 (4%)	6 (2%)	7	20
1	E	378/387 (98%)	359 (95%)	12 (3%)	7 (2%)	6	17
1	F	378/387 (98%)	358 (95%)	14 (4%)	6 (2%)	7	20
1	G	378/387 (98%)	356 (94%)	16 (4%)	6 (2%)	7	20
1	H	378/387 (98%)	359 (95%)	13 (3%)	6 (2%)	7	20
1	I	378/387 (98%)	356 (94%)	15 (4%)	7 (2%)	6	17
1	J	378/387 (98%)	352 (93%)	19 (5%)	7 (2%)	6	17
1	K	378/387 (98%)	358 (95%)	12 (3%)	8 (2%)	5	15
1	L	378/387 (98%)	360 (95%)	11 (3%)	7 (2%)	6	17
1	M	378/387 (98%)	363 (96%)	9 (2%)	6 (2%)	7	20
1	N	378/387 (98%)	359 (95%)	13 (3%)	6 (2%)	7	20
1	O	378/387 (98%)	360 (95%)	12 (3%)	6 (2%)	7	20
1	P	378/387 (98%)	354 (94%)	19 (5%)	5 (1%)	9	25
1	Q	378/387 (98%)	358 (95%)	16 (4%)	4 (1%)	11	29
1	R	378/387 (98%)	363 (96%)	11 (3%)	4 (1%)	11	29
1	S	378/387 (98%)	352 (93%)	15 (4%)	11 (3%)	3	9
1	T	378/387 (98%)	356 (94%)	18 (5%)	4 (1%)	11	29
All	All	7560/7740 (98%)	7154 (95%)	280 (4%)	126 (2%)	7	19

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP

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Mol	Chain	Res	Type
1	A	127	ILE
1	B	120	ASP
1	B	127	ILE
1	D	120	ASP
1	D	127	ILE
1	E	120	ASP
1	E	127	ILE
1	F	127	ILE
1	H	75	ASN
1	H	120	ASP
1	H	121	LEU
1	I	120	ASP
1	J	119	GLY
1	K	49	ASP
1	K	120	ASP
1	K	121	LEU
1	K	127	ILE
1	L	119	GLY
1	L	128	GLU
1	M	118	GLU
1	M	120	ASP
1	M	121	LEU
1	N	127	ILE
1	O	119	GLY
1	O	127	ILE
1	P	127	ILE
1	Q	119	GLY
1	Q	127	ILE
1	R	127	ILE
1	S	119	GLY
1	S	281	HIS
1	T	127	ILE
1	B	50	GLY
1	B	145	GLY
1	C	50	GLY
1	C	119	GLY
1	C	128	GLU
1	C	316	THR
1	D	119	GLY
1	E	119	GLY
1	E	278	ASP
1	G	50	GLY

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Mol	Chain	Res	Type
1	G	119	GLY
1	G	127	ILE
1	G	145	GLY
1	H	145	GLY
1	H	278	ASP
1	I	127	ILE
1	I	128	GLU
1	I	145	GLY
1	J	127	ILE
1	J	128	GLU
1	J	145	GLY
1	L	50	GLY
1	L	127	ILE
1	M	119	GLY
1	N	118	GLU
1	O	145	GLY
1	Q	51	ALA
1	R	49	ASP
1	A	119	GLY
1	B	119	GLY
1	C	92	GLN
1	C	145	GLY
1	D	50	GLY
1	E	51	ALA
1	E	145	GLY
1	F	145	GLY
1	I	119	GLY
1	J	49	ASP
1	L	121	LEU
1	L	145	GLY
1	M	145	GLY
1	N	145	GLY
1	P	145	GLY
1	R	50	GLY
1	R	145	GLY
1	S	49	ASP
1	S	118	GLU
1	S	278	ASP
1	T	50	GLY
1	A	121	LEU
1	A	145	GLY
1	D	145	GLY

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Mol	Chain	Res	Type
1	F	50	GLY
1	F	119	GLY
1	G	128	GLU
1	H	50	GLY
1	K	50	GLY
1	K	128	GLU
1	L	120	ASP
1	N	119	GLY
1	N	120	ASP
1	O	50	GLY
1	O	278	ASP
1	P	51	ALA
1	P	120	ASP
1	Q	145	GLY
1	S	127	ILE
1	T	145	GLY
1	B	49	ASP
1	D	51	ALA
1	F	120	ASP
1	F	278	ASP
1	I	162	LYS
1	K	145	GLY
1	M	50	GLY
1	S	50	GLY
1	S	128	GLU
1	S	145	GLY
1	S	353	ASP
1	A	50	GLY
1	A	316	THR
1	G	75	ASN
1	N	50	GLY
1	B	75	ASN
1	J	50	GLY
1	P	50	GLY
1	S	75	ASN
1	T	75	ASN
1	J	75	ASN
1	E	75	ASN
1	K	75	ASN
1	O	75	ASN
1	I	50	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	296/302 (98%)	260 (88%)	36 (12%)	5	12
1	B	296/302 (98%)	256 (86%)	40 (14%)	4	9
1	C	296/302 (98%)	263 (89%)	33 (11%)	6	15
1	D	296/302 (98%)	247 (83%)	49 (17%)	2	6
1	E	296/302 (98%)	247 (83%)	49 (17%)	2	6
1	F	296/302 (98%)	263 (89%)	33 (11%)	6	15
1	G	296/302 (98%)	255 (86%)	41 (14%)	3	9
1	H	296/302 (98%)	251 (85%)	45 (15%)	3	7
1	I	296/302 (98%)	255 (86%)	41 (14%)	3	9
1	J	296/302 (98%)	258 (87%)	38 (13%)	4	11
1	K	296/302 (98%)	253 (86%)	43 (14%)	3	8
1	L	296/302 (98%)	255 (86%)	41 (14%)	3	9
1	M	296/302 (98%)	256 (86%)	40 (14%)	4	9
1	N	296/302 (98%)	262 (88%)	34 (12%)	5	14
1	O	296/302 (98%)	254 (86%)	42 (14%)	3	8
1	P	296/302 (98%)	246 (83%)	50 (17%)	2	6
1	Q	296/302 (98%)	247 (83%)	49 (17%)	2	6
1	R	296/302 (98%)	257 (87%)	39 (13%)	4	10
1	S	296/302 (98%)	261 (88%)	35 (12%)	5	13
1	T	296/302 (98%)	264 (89%)	32 (11%)	6	16
All	All	5920/6040 (98%)	5110 (86%)	810 (14%)	3	9

All (810) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	49	ASP
1	A	56	LEU

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	66	VAL
1	A	68	ILE
1	A	116	THR
1	A	121	LEU
1	A	127	ILE
1	A	131	THR
1	A	140	VAL
1	A	146	THR
1	A	150	VAL
1	A	151	THR
1	A	155	VAL
1	A	156	LEU
1	A	160	GLU
1	A	171	ARG
1	A	173	LEU
1	A	182	LEU
1	A	191	LEU
1	A	192	THR
1	A	200	LEU
1	A	204	VAL
1	A	213	ASN
1	A	216	THR
1	A	222	GLN
1	A	233	GLN
1	A	244	ARG
1	A	288	LEU
1	A	289	LEU
1	A	310	LEU
1	A	332	THR
1	A	333	ARG
1	A	362	LEU
1	A	375	ASN
1	B	24	VAL
1	B	38	LEU
1	B	49	ASP
1	B	56	LEU
1	B	59	LEU
1	B	65	GLU
1	B	68	ILE
1	B	99	VAL
1	B	116	THR

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Mol	Chain	Res	Type
1	B	121	LEU
1	B	127	ILE
1	B	128	GLU
1	B	130	LEU
1	B	131	THR
1	B	140	VAL
1	B	143	THR
1	B	150	VAL
1	B	151	THR
1	B	155	VAL
1	B	156	LEU
1	B	173	LEU
1	B	182	LEU
1	B	191	LEU
1	B	192	THR
1	B	200	LEU
1	B	204	VAL
1	B	216	THR
1	B	222	GLN
1	B	233	GLN
1	B	235	VAL
1	B	241	LEU
1	B	244	ARG
1	B	283	VAL
1	B	287	VAL
1	B	288	LEU
1	B	289	LEU
1	B	310	LEU
1	B	332	THR
1	B	333	ARG
1	B	375	ASN
1	C	49	ASP
1	C	59	LEU
1	C	68	ILE
1	C	99	VAL
1	C	116	THR
1	C	120	ASP
1	C	127	ILE
1	C	128	GLU
1	C	131	THR
1	C	140	VAL
1	C	143	THR

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Mol	Chain	Res	Type
1	C	150	VAL
1	C	155	VAL
1	C	173	LEU
1	C	182	LEU
1	C	191	LEU
1	C	192	THR
1	C	200	LEU
1	C	213	ASN
1	C	216	THR
1	C	222	GLN
1	C	233	GLN
1	C	235	VAL
1	C	241	LEU
1	C	244	ARG
1	C	258	PHE
1	C	288	LEU
1	C	289	LEU
1	C	310	LEU
1	C	332	THR
1	C	333	ARG
1	C	362	LEU
1	C	375	ASN
1	D	24	VAL
1	D	38	LEU
1	D	45	ARG
1	D	48	LYS
1	D	49	ASP
1	D	55	THR
1	D	56	LEU
1	D	60	ARG
1	D	61	GLU
1	D	68	ILE
1	D	99	VAL
1	D	116	THR
1	D	121	LEU
1	D	128	GLU
1	D	130	LEU
1	D	131	THR
1	D	140	VAL
1	D	146	THR
1	D	150	VAL
1	D	151	THR

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Mol	Chain	Res	Type
1	D	156	LEU
1	D	173	LEU
1	D	175	SER
1	D	182	LEU
1	D	183	LEU
1	D	185	ILE
1	D	191	LEU
1	D	192	THR
1	D	200	LEU
1	D	204	VAL
1	D	213	ASN
1	D	216	THR
1	D	222	GLN
1	D	233	GLN
1	D	235	VAL
1	D	241	LEU
1	D	244	ARG
1	D	258	PHE
1	D	283	VAL
1	D	288	LEU
1	D	289	LEU
1	D	310	LEU
1	D	315	ILE
1	D	332	THR
1	D	333	ARG
1	D	347	LEU
1	D	362	LEU
1	D	375	ASN
1	D	377	GLN
1	E	10	VAL
1	E	24	VAL
1	E	38	LEU
1	E	45	ARG
1	E	55	THR
1	E	56	LEU
1	E	59	LEU
1	E	64	ILE
1	E	65	GLU
1	E	68	ILE
1	E	99	VAL
1	E	116	THR
1	E	120	ASP

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Mol	Chain	Res	Type
1	E	121	LEU
1	E	127	ILE
1	E	128	GLU
1	E	130	LEU
1	E	140	VAL
1	E	142	THR
1	E	143	THR
1	E	150	VAL
1	E	151	THR
1	E	152	ARG
1	E	155	VAL
1	E	156	LEU
1	E	173	LEU
1	E	182	LEU
1	E	183	LEU
1	E	191	LEU
1	E	192	THR
1	E	200	LEU
1	E	204	VAL
1	E	216	THR
1	E	222	GLN
1	E	233	GLN
1	E	235	VAL
1	E	241	LEU
1	E	244	ARG
1	E	258	PHE
1	E	283	VAL
1	E	288	LEU
1	E	289	LEU
1	E	310	LEU
1	E	315	ILE
1	E	332	THR
1	E	333	ARG
1	E	347	LEU
1	E	362	LEU
1	E	375	ASN
1	F	38	LEU
1	F	41	ASP
1	F	49	ASP
1	F	55	THR
1	F	56	LEU
1	F	68	ILE

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Mol	Chain	Res	Type
1	F	82	ARG
1	F	116	THR
1	F	121	LEU
1	F	127	ILE
1	F	130	LEU
1	F	131	THR
1	F	140	VAL
1	F	143	THR
1	F	150	VAL
1	F	151	THR
1	F	155	VAL
1	F	173	LEU
1	F	183	LEU
1	F	191	LEU
1	F	192	THR
1	F	200	LEU
1	F	204	VAL
1	F	216	THR
1	F	222	GLN
1	F	233	GLN
1	F	241	LEU
1	F	244	ARG
1	F	288	LEU
1	F	289	LEU
1	F	310	LEU
1	F	347	LEU
1	F	375	ASN
1	G	10	VAL
1	G	24	VAL
1	G	38	LEU
1	G	49	ASP
1	G	55	THR
1	G	59	LEU
1	G	65	GLU
1	G	68	ILE
1	G	99	VAL
1	G	116	THR
1	G	127	ILE
1	G	128	GLU
1	G	140	VAL
1	G	143	THR
1	G	146	THR

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Mol	Chain	Res	Type
1	G	150	VAL
1	G	151	THR
1	G	152	ARG
1	G	155	VAL
1	G	159	THR
1	G	173	LEU
1	G	182	LEU
1	G	183	LEU
1	G	191	LEU
1	G	192	THR
1	G	200	LEU
1	G	204	VAL
1	G	213	ASN
1	G	216	THR
1	G	222	GLN
1	G	233	GLN
1	G	235	VAL
1	G	241	LEU
1	G	244	ARG
1	G	288	LEU
1	G	289	LEU
1	G	310	LEU
1	G	332	THR
1	G	333	ARG
1	G	362	LEU
1	G	375	ASN
1	H	12	ASN
1	H	24	VAL
1	H	38	LEU
1	H	45	ARG
1	H	49	ASP
1	H	55	THR
1	H	56	LEU
1	H	64	ILE
1	H	68	ILE
1	H	75	ASN
1	H	99	VAL
1	H	121	LEU
1	H	128	GLU
1	H	131	THR
1	H	140	VAL
1	H	143	THR

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Mol	Chain	Res	Type
1	H	150	VAL
1	H	151	THR
1	H	152	ARG
1	H	155	VAL
1	H	156	LEU
1	H	171	ARG
1	H	173	LEU
1	H	182	LEU
1	H	183	LEU
1	H	191	LEU
1	H	192	THR
1	H	200	LEU
1	H	204	VAL
1	H	213	ASN
1	H	216	THR
1	H	222	GLN
1	H	233	GLN
1	H	235	VAL
1	H	241	LEU
1	H	244	ARG
1	H	258	PHE
1	H	288	LEU
1	H	289	LEU
1	H	310	LEU
1	H	315	ILE
1	H	332	THR
1	H	333	ARG
1	H	362	LEU
1	H	375	ASN
1	I	38	LEU
1	I	55	THR
1	I	56	LEU
1	I	68	ILE
1	I	116	THR
1	I	120	ASP
1	I	121	LEU
1	I	128	GLU
1	I	140	VAL
1	I	150	VAL
1	I	151	THR
1	I	152	ARG
1	I	155	VAL

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Mol	Chain	Res	Type
1	I	156	LEU
1	I	173	LEU
1	I	182	LEU
1	I	183	LEU
1	I	191	LEU
1	I	192	THR
1	I	200	LEU
1	I	204	VAL
1	I	213	ASN
1	I	216	THR
1	I	222	GLN
1	I	233	GLN
1	I	235	VAL
1	I	241	LEU
1	I	242	GLN
1	I	244	ARG
1	I	258	PHE
1	I	278	ASP
1	I	288	LEU
1	I	289	LEU
1	I	310	LEU
1	I	332	THR
1	I	333	ARG
1	I	347	LEU
1	I	352	THR
1	I	359	GLU
1	I	362	LEU
1	I	375	ASN
1	J	24	VAL
1	J	45	ARG
1	J	49	ASP
1	J	55	THR
1	J	59	LEU
1	J	64	ILE
1	J	68	ILE
1	J	116	THR
1	J	121	LEU
1	J	127	ILE
1	J	128	GLU
1	J	130	LEU
1	J	140	VAL
1	J	142	THR

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Mol	Chain	Res	Type
1	J	143	THR
1	J	150	VAL
1	J	151	THR
1	J	160	GLU
1	J	173	LEU
1	J	182	LEU
1	J	183	LEU
1	J	191	LEU
1	J	192	THR
1	J	200	LEU
1	J	213	ASN
1	J	222	GLN
1	J	233	GLN
1	J	235	VAL
1	J	241	LEU
1	J	244	ARG
1	J	252	LEU
1	J	283	VAL
1	J	289	LEU
1	J	310	LEU
1	J	332	THR
1	J	333	ARG
1	J	347	LEU
1	J	375	ASN
1	K	24	VAL
1	K	45	ARG
1	K	55	THR
1	K	56	LEU
1	K	64	ILE
1	K	68	ILE
1	K	99	VAL
1	K	116	THR
1	K	121	LEU
1	K	127	ILE
1	K	128	GLU
1	K	130	LEU
1	K	131	THR
1	K	140	VAL
1	K	143	THR
1	K	150	VAL
1	K	151	THR
1	K	155	VAL

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Mol	Chain	Res	Type
1	K	156	LEU
1	K	173	LEU
1	K	182	LEU
1	K	183	LEU
1	K	191	LEU
1	K	192	THR
1	K	200	LEU
1	K	204	VAL
1	K	216	THR
1	K	222	GLN
1	K	233	GLN
1	K	235	VAL
1	K	241	LEU
1	K	242	GLN
1	K	244	ARG
1	K	283	VAL
1	K	287	VAL
1	K	288	LEU
1	K	289	LEU
1	K	310	LEU
1	K	332	THR
1	K	333	ARG
1	K	347	LEU
1	K	362	LEU
1	K	375	ASN
1	L	10	VAL
1	L	38	LEU
1	L	41	ASP
1	L	49	ASP
1	L	55	THR
1	L	65	GLU
1	L	68	ILE
1	L	75	ASN
1	L	116	THR
1	L	121	LEU
1	L	128	GLU
1	L	131	THR
1	L	140	VAL
1	L	143	THR
1	L	150	VAL
1	L	151	THR
1	L	155	VAL

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Mol	Chain	Res	Type
1	L	156	LEU
1	L	173	LEU
1	L	182	LEU
1	L	191	LEU
1	L	192	THR
1	L	200	LEU
1	L	204	VAL
1	L	213	ASN
1	L	216	THR
1	L	222	GLN
1	L	233	GLN
1	L	235	VAL
1	L	241	LEU
1	L	244	ARG
1	L	258	PHE
1	L	288	LEU
1	L	289	LEU
1	L	310	LEU
1	L	332	THR
1	L	333	ARG
1	L	347	LEU
1	L	352	THR
1	L	362	LEU
1	L	375	ASN
1	M	24	VAL
1	M	38	LEU
1	M	45	ARG
1	M	49	ASP
1	M	55	THR
1	M	59	LEU
1	M	68	ILE
1	M	99	VAL
1	M	118	GLU
1	M	121	LEU
1	M	128	GLU
1	M	140	VAL
1	M	143	THR
1	M	150	VAL
1	M	155	VAL
1	M	156	LEU
1	M	173	LEU
1	M	182	LEU

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Mol	Chain	Res	Type
1	M	183	LEU
1	M	191	LEU
1	M	192	THR
1	M	200	LEU
1	M	204	VAL
1	M	216	THR
1	M	222	GLN
1	M	233	GLN
1	M	235	VAL
1	M	241	LEU
1	M	244	ARG
1	M	258	PHE
1	M	283	VAL
1	M	288	LEU
1	M	289	LEU
1	M	310	LEU
1	M	315	ILE
1	M	332	THR
1	M	333	ARG
1	M	347	LEU
1	M	362	LEU
1	M	375	ASN
1	N	38	LEU
1	N	48	LYS
1	N	49	ASP
1	N	55	THR
1	N	99	VAL
1	N	120	ASP
1	N	121	LEU
1	N	122	TYR
1	N	127	ILE
1	N	140	VAL
1	N	142	THR
1	N	143	THR
1	N	150	VAL
1	N	151	THR
1	N	173	LEU
1	N	182	LEU
1	N	191	LEU
1	N	192	THR
1	N	200	LEU
1	N	204	VAL

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Mol	Chain	Res	Type
1	N	213	ASN
1	N	216	THR
1	N	222	GLN
1	N	233	GLN
1	N	235	VAL
1	N	241	LEU
1	N	244	ARG
1	N	278	ASP
1	N	289	LEU
1	N	310	LEU
1	N	332	THR
1	N	333	ARG
1	N	362	LEU
1	N	375	ASN
1	O	24	VAL
1	O	38	LEU
1	O	48	LYS
1	O	49	ASP
1	O	55	THR
1	O	59	LEU
1	O	66	VAL
1	O	68	ILE
1	O	82	ARG
1	O	118	GLU
1	O	127	ILE
1	O	128	GLU
1	O	130	LEU
1	O	131	THR
1	O	140	VAL
1	O	143	THR
1	O	150	VAL
1	O	151	THR
1	O	152	ARG
1	O	171	ARG
1	O	173	LEU
1	O	182	LEU
1	O	183	LEU
1	O	191	LEU
1	O	192	THR
1	O	200	LEU
1	O	204	VAL
1	O	213	ASN

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Mol	Chain	Res	Type
1	O	216	THR
1	O	222	GLN
1	O	233	GLN
1	O	235	VAL
1	O	241	LEU
1	O	288	LEU
1	O	289	LEU
1	O	310	LEU
1	O	332	THR
1	O	333	ARG
1	O	347	LEU
1	O	352	THR
1	O	362	LEU
1	O	375	ASN
1	P	5	MET
1	P	24	VAL
1	P	38	LEU
1	P	45	ARG
1	P	48	LYS
1	P	52	VAL
1	P	55	THR
1	P	56	LEU
1	P	59	LEU
1	P	66	VAL
1	P	68	ILE
1	P	94	ASP
1	P	99	VAL
1	P	116	THR
1	P	120	ASP
1	P	121	LEU
1	P	127	ILE
1	P	128	GLU
1	P	130	LEU
1	P	131	THR
1	P	140	VAL
1	P	142	THR
1	P	143	THR
1	P	150	VAL
1	P	151	THR
1	P	155	VAL
1	P	156	LEU
1	P	173	LEU

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Mol	Chain	Res	Type
1	P	182	LEU
1	P	183	LEU
1	P	191	LEU
1	P	192	THR
1	P	200	LEU
1	P	204	VAL
1	P	213	ASN
1	P	216	THR
1	P	222	GLN
1	P	233	GLN
1	P	235	VAL
1	P	241	LEU
1	P	244	ARG
1	P	278	ASP
1	P	283	VAL
1	P	288	LEU
1	P	289	LEU
1	P	310	LEU
1	P	332	THR
1	P	333	ARG
1	P	347	LEU
1	P	375	ASN
1	Q	9	LEU
1	Q	24	VAL
1	Q	38	LEU
1	Q	45	ARG
1	Q	52	VAL
1	Q	55	THR
1	Q	56	LEU
1	Q	59	LEU
1	Q	68	ILE
1	Q	99	VAL
1	Q	121	LEU
1	Q	123	GLN
1	Q	127	ILE
1	Q	128	GLU
1	Q	130	LEU
1	Q	131	THR
1	Q	140	VAL
1	Q	143	THR
1	Q	148	SER
1	Q	150	VAL

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Mol	Chain	Res	Type
1	Q	151	THR
1	Q	155	VAL
1	Q	156	LEU
1	Q	173	LEU
1	Q	175	SER
1	Q	182	LEU
1	Q	183	LEU
1	Q	191	LEU
1	Q	192	THR
1	Q	200	LEU
1	Q	204	VAL
1	Q	213	ASN
1	Q	216	THR
1	Q	222	GLN
1	Q	233	GLN
1	Q	235	VAL
1	Q	241	LEU
1	Q	244	ARG
1	Q	258	PHE
1	Q	283	VAL
1	Q	288	LEU
1	Q	289	LEU
1	Q	310	LEU
1	Q	315	ILE
1	Q	332	THR
1	Q	333	ARG
1	Q	347	LEU
1	Q	362	LEU
1	Q	375	ASN
1	R	38	LEU
1	R	49	ASP
1	R	55	THR
1	R	68	ILE
1	R	99	VAL
1	R	116	THR
1	R	127	ILE
1	R	130	LEU
1	R	131	THR
1	R	140	VAL
1	R	143	THR
1	R	150	VAL
1	R	151	THR

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Mol	Chain	Res	Type
1	R	152	ARG
1	R	156	LEU
1	R	160	GLU
1	R	173	LEU
1	R	182	LEU
1	R	183	LEU
1	R	191	LEU
1	R	200	LEU
1	R	204	VAL
1	R	213	ASN
1	R	216	THR
1	R	222	GLN
1	R	233	GLN
1	R	235	VAL
1	R	241	LEU
1	R	244	ARG
1	R	258	PHE
1	R	283	VAL
1	R	288	LEU
1	R	289	LEU
1	R	310	LEU
1	R	325	GLU
1	R	332	THR
1	R	333	ARG
1	R	362	LEU
1	R	375	ASN
1	S	24	VAL
1	S	38	LEU
1	S	49	ASP
1	S	56	LEU
1	S	79	THR
1	S	99	VAL
1	S	116	THR
1	S	121	LEU
1	S	127	ILE
1	S	128	GLU
1	S	130	LEU
1	S	140	VAL
1	S	143	THR
1	S	151	THR
1	S	152	ARG
1	S	183	LEU

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Mol	Chain	Res	Type
1	S	191	LEU
1	S	200	LEU
1	S	213	ASN
1	S	216	THR
1	S	222	GLN
1	S	233	GLN
1	S	235	VAL
1	S	241	LEU
1	S	244	ARG
1	S	258	PHE
1	S	288	LEU
1	S	289	LEU
1	S	310	LEU
1	S	315	ILE
1	S	332	THR
1	S	333	ARG
1	S	347	LEU
1	S	362	LEU
1	S	375	ASN
1	T	10	VAL
1	T	24	VAL
1	T	38	LEU
1	T	49	ASP
1	T	56	LEU
1	T	59	LEU
1	T	68	ILE
1	T	116	THR
1	T	121	LEU
1	T	127	ILE
1	T	128	GLU
1	T	140	VAL
1	T	155	VAL
1	T	156	LEU
1	T	191	LEU
1	T	192	THR
1	T	200	LEU
1	T	204	VAL
1	T	213	ASN
1	T	222	GLN
1	T	233	GLN
1	T	235	VAL
1	T	241	LEU

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Mol	Chain	Res	Type
1	T	258	PHE
1	T	288	LEU
1	T	289	LEU
1	T	310	LEU
1	T	332	THR
1	T	333	ARG
1	T	362	LEU
1	T	375	ASN
1	T	384	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (342) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	29	GLN
1	A	75	ASN
1	A	92	GLN
1	A	105	HIS
1	A	141	ASN
1	A	172	ASN
1	A	213	ASN
1	A	222	GLN
1	A	233	GLN
1	A	242	GLN
1	A	259	ASN
1	A	260	ASN
1	A	271	HIS
1	A	285	ASN
1	A	343	HIS
1	A	366	ASN
1	A	370	ASN
1	A	375	ASN
1	B	14	ASN
1	B	29	GLN
1	B	75	ASN
1	B	105	HIS
1	B	141	ASN
1	B	153	HIS
1	B	172	ASN
1	B	213	ASN
1	B	222	GLN
1	B	233	GLN

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Mol	Chain	Res	Type
1	B	242	GLN
1	B	259	ASN
1	B	260	ASN
1	B	285	ASN
1	B	291	HIS
1	B	370	ASN
1	B	375	ASN
1	B	385	GLN
1	C	14	ASN
1	C	29	GLN
1	C	75	ASN
1	C	141	ASN
1	C	153	HIS
1	C	172	ASN
1	C	213	ASN
1	C	222	GLN
1	C	233	GLN
1	C	259	ASN
1	C	260	ASN
1	C	271	HIS
1	C	285	ASN
1	C	291	HIS
1	C	342	GLN
1	C	370	ASN
1	C	375	ASN
1	C	385	GLN
1	D	14	ASN
1	D	29	GLN
1	D	153	HIS
1	D	172	ASN
1	D	213	ASN
1	D	222	GLN
1	D	233	GLN
1	D	259	ASN
1	D	260	ASN
1	D	285	ASN
1	D	291	HIS
1	D	366	ASN
1	D	370	ASN
1	D	375	ASN
1	D	385	GLN
1	E	29	GLN

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Mol	Chain	Res	Type
1	E	75	ASN
1	E	92	GLN
1	E	105	HIS
1	E	123	GLN
1	E	141	ASN
1	E	153	HIS
1	E	172	ASN
1	E	213	ASN
1	E	222	GLN
1	E	233	GLN
1	E	259	ASN
1	E	260	ASN
1	E	285	ASN
1	E	342	GLN
1	E	343	HIS
1	E	370	ASN
1	E	375	ASN
1	F	80	ASN
1	F	123	GLN
1	F	172	ASN
1	F	213	ASN
1	F	222	GLN
1	F	233	GLN
1	F	242	GLN
1	F	259	ASN
1	F	260	ASN
1	F	271	HIS
1	F	285	ASN
1	F	366	ASN
1	F	370	ASN
1	F	375	ASN
1	F	385	GLN
1	G	14	ASN
1	G	29	GLN
1	G	75	ASN
1	G	105	HIS
1	G	153	HIS
1	G	158	ASN
1	G	172	ASN
1	G	213	ASN
1	G	222	GLN
1	G	233	GLN

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Mol	Chain	Res	Type
1	G	259	ASN
1	G	260	ASN
1	G	285	ASN
1	G	342	GLN
1	G	370	ASN
1	G	375	ASN
1	G	385	GLN
1	H	29	GLN
1	H	75	ASN
1	H	92	GLN
1	H	105	HIS
1	H	132	ASN
1	H	172	ASN
1	H	213	ASN
1	H	222	GLN
1	H	233	GLN
1	H	259	ASN
1	H	260	ASN
1	H	271	HIS
1	H	285	ASN
1	H	291	HIS
1	H	370	ASN
1	H	375	ASN
1	H	385	GLN
1	I	14	ASN
1	I	29	GLN
1	I	105	HIS
1	I	123	GLN
1	I	141	ASN
1	I	153	HIS
1	I	179	ASN
1	I	213	ASN
1	I	222	GLN
1	I	233	GLN
1	I	259	ASN
1	I	260	ASN
1	I	271	HIS
1	I	285	ASN
1	I	291	HIS
1	I	300	ASN
1	I	343	HIS
1	I	366	ASN

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Mol	Chain	Res	Type
1	I	370	ASN
1	I	375	ASN
1	J	14	ASN
1	J	29	GLN
1	J	75	ASN
1	J	105	HIS
1	J	123	GLN
1	J	213	ASN
1	J	222	GLN
1	J	233	GLN
1	J	242	GLN
1	J	259	ASN
1	J	260	ASN
1	J	271	HIS
1	J	285	ASN
1	J	366	ASN
1	J	370	ASN
1	J	375	ASN
1	J	385	GLN
1	K	29	GLN
1	K	75	ASN
1	K	105	HIS
1	K	123	GLN
1	K	141	ASN
1	K	172	ASN
1	K	213	ASN
1	K	222	GLN
1	K	233	GLN
1	K	259	ASN
1	K	260	ASN
1	K	271	HIS
1	K	285	ASN
1	K	291	HIS
1	K	342	GLN
1	K	370	ASN
1	K	375	ASN
1	L	14	ASN
1	L	29	GLN
1	L	75	ASN
1	L	105	HIS
1	L	141	ASN
1	L	153	HIS

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Mol	Chain	Res	Type
1	L	158	ASN
1	L	213	ASN
1	L	222	GLN
1	L	233	GLN
1	L	259	ASN
1	L	260	ASN
1	L	285	ASN
1	L	370	ASN
1	L	375	ASN
1	L	385	GLN
1	M	29	GLN
1	M	105	HIS
1	M	123	GLN
1	M	141	ASN
1	M	172	ASN
1	M	213	ASN
1	M	222	GLN
1	M	233	GLN
1	M	242	GLN
1	M	259	ASN
1	M	260	ASN
1	M	285	ASN
1	M	366	ASN
1	M	370	ASN
1	M	375	ASN
1	M	385	GLN
1	N	14	ASN
1	N	29	GLN
1	N	75	ASN
1	N	141	ASN
1	N	172	ASN
1	N	213	ASN
1	N	222	GLN
1	N	233	GLN
1	N	259	ASN
1	N	260	ASN
1	N	271	HIS
1	N	285	ASN
1	N	342	GLN
1	N	343	HIS
1	N	370	ASN
1	N	375	ASN

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Mol	Chain	Res	Type
1	N	385	GLN
1	O	14	ASN
1	O	29	GLN
1	O	75	ASN
1	O	105	HIS
1	O	141	ASN
1	O	153	HIS
1	O	172	ASN
1	O	213	ASN
1	O	222	GLN
1	O	233	GLN
1	O	259	ASN
1	O	260	ASN
1	O	285	ASN
1	O	291	HIS
1	O	366	ASN
1	O	370	ASN
1	O	375	ASN
1	P	14	ASN
1	P	29	GLN
1	P	75	ASN
1	P	105	HIS
1	P	123	GLN
1	P	153	HIS
1	P	172	ASN
1	P	179	ASN
1	P	213	ASN
1	P	222	GLN
1	P	233	GLN
1	P	259	ASN
1	P	260	ASN
1	P	271	HIS
1	P	285	ASN
1	P	291	HIS
1	P	370	ASN
1	P	375	ASN
1	P	385	GLN
1	Q	14	ASN
1	Q	29	GLN
1	Q	75	ASN
1	Q	105	HIS
1	Q	123	GLN

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Mol	Chain	Res	Type
1	Q	141	ASN
1	Q	153	HIS
1	Q	172	ASN
1	Q	213	ASN
1	Q	222	GLN
1	Q	233	GLN
1	Q	259	ASN
1	Q	260	ASN
1	Q	285	ASN
1	Q	291	HIS
1	Q	343	HIS
1	Q	366	ASN
1	Q	370	ASN
1	Q	375	ASN
1	R	14	ASN
1	R	29	GLN
1	R	80	ASN
1	R	105	HIS
1	R	141	ASN
1	R	172	ASN
1	R	213	ASN
1	R	222	GLN
1	R	233	GLN
1	R	259	ASN
1	R	260	ASN
1	R	285	ASN
1	R	370	ASN
1	R	375	ASN
1	S	29	GLN
1	S	75	ASN
1	S	105	HIS
1	S	141	ASN
1	S	179	ASN
1	S	202	HIS
1	S	213	ASN
1	S	222	GLN
1	S	233	GLN
1	S	259	ASN
1	S	260	ASN
1	S	271	HIS
1	S	285	ASN
1	S	370	ASN

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Mol	Chain	Res	Type
1	S	375	ASN
1	S	385	GLN
1	T	14	ASN
1	T	29	GLN
1	T	80	ASN
1	T	92	GLN
1	T	141	ASN
1	T	172	ASN
1	T	213	ASN
1	T	222	GLN
1	T	233	GLN
1	T	259	ASN
1	T	260	ASN
1	T	271	HIS
1	T	285	ASN
1	T	366	ASN
1	T	370	ASN
1	T	375	ASN
1	T	385	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 20 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

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, 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	382/387 (98%)	0.30	10 (2%) 57 54	41, 46, 51, 57	0
1	B	382/387 (98%)	0.04	6 (1%) 70 68	39, 45, 51, 56	0
1	C	382/387 (98%)	0.23	6 (1%) 70 68	41, 46, 51, 55	0
1	D	382/387 (98%)	0.17	6 (1%) 70 68	39, 46, 51, 56	0
1	E	382/387 (98%)	0.08	11 (2%) 53 50	40, 45, 51, 56	0
1	F	382/387 (98%)	0.44	12 (3%) 51 48	41, 46, 51, 56	0
1	G	382/387 (98%)	0.21	9 (2%) 59 56	41, 45, 51, 57	0
1	H	382/387 (98%)	0.27	12 (3%) 51 48	39, 45, 51, 58	0
1	I	382/387 (98%)	0.63	26 (6%) 23 20	40, 46, 51, 55	0
1	J	382/387 (98%)	0.14	7 (1%) 67 65	41, 46, 51, 56	0
1	K	382/387 (98%)	0.18	11 (2%) 53 50	39, 45, 51, 59	0
1	L	382/387 (98%)	0.57	19 (4%) 34 30	41, 46, 51, 58	0
1	M	382/387 (98%)	0.18	7 (1%) 67 65	39, 45, 50, 57	0
1	N	382/387 (98%)	0.40	12 (3%) 51 48	41, 46, 51, 55	0
1	O	382/387 (98%)	0.16	10 (2%) 57 54	40, 45, 51, 58	0
1	P	382/387 (98%)	0.04	7 (1%) 67 65	40, 45, 50, 56	0
1	Q	382/387 (98%)	0.08	6 (1%) 70 68	39, 46, 50, 55	0
1	R	382/387 (98%)	0.45	11 (2%) 53 50	41, 46, 50, 57	0
1	S	382/387 (98%)	0.74	26 (6%) 23 20	41, 46, 51, 58	0
1	T	382/387 (98%)	0.48	21 (5%) 30 27	40, 46, 50, 55	0
All	All	7640/7740 (98%)	0.29	235 (3%) 51 48	39, 46, 51, 59	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	4.1
1	H	50	GLY	3.9
1	I	278	ASP	3.9
1	I	121	LEU	3.8
1	Q	121	LEU	3.8
1	C	51	ALA	3.8
1	F	6	PHE	3.7
1	L	352	THR	3.6
1	I	49	ASP	3.6
1	D	122	TYR	3.6
1	S	50	GLY	3.6
1	M	121	LEU	3.6
1	H	352	THR	3.6
1	H	51	ALA	3.6
1	D	50	GLY	3.5
1	P	50	GLY	3.5
1	F	49	ASP	3.5
1	L	50	GLY	3.5
1	S	94	ASP	3.4
1	Q	51	ALA	3.4
1	A	6	PHE	3.4
1	S	119	GLY	3.3
1	H	246	TYR	3.3
1	O	352	THR	3.3
1	A	49	ASP	3.3
1	O	50	GLY	3.3
1	O	127	ILE	3.3
1	F	352	THR	3.3
1	G	4	ARG	3.2
1	D	121	LEU	3.2
1	E	121	LEU	3.2
1	E	127	ILE	3.2
1	R	127	ILE	3.2
1	T	68	ILE	3.2
1	K	121	LEU	3.2
1	I	215	VAL	3.2
1	G	48	LYS	3.1
1	R	49	ASP	3.1
1	K	127	ILE	3.1
1	T	156	LEU	3.1
1	S	6	PHE	3.1
1	A	121	LEU	3.1
1	A	50	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	T	100	GLY	3.1
1	S	113	ILE	3.1
1	T	352	THR	3.0
1	L	48	LYS	3.0
1	D	127	ILE	3.0
1	S	352	THR	3.0
1	E	48	LYS	3.0
1	E	50	GLY	3.0
1	L	121	LEU	2.9
1	C	49	ASP	2.9
1	P	127	ILE	2.9
1	O	48	LYS	2.9
1	P	368	PHE	2.9
1	H	48	LYS	2.9
1	B	49	ASP	2.8
1	L	68	ILE	2.8
1	N	50	GLY	2.8
1	T	368	PHE	2.8
1	I	41	ASP	2.8
1	Q	127	ILE	2.8
1	N	121	LEU	2.8
1	E	278	ASP	2.8
1	I	6	PHE	2.8
1	T	121	LEU	2.7
1	E	49	ASP	2.7
1	K	118	GLU	2.7
1	L	120	ASP	2.7
1	A	315	ILE	2.7
1	L	144	ALA	2.7
1	B	127	ILE	2.7
1	I	5	MET	2.7
1	C	50	GLY	2.7
1	J	278	ASP	2.7
1	T	142	THR	2.7
1	P	48	LYS	2.7
1	P	82	ARG	2.6
1	L	51	ALA	2.6
1	L	368	PHE	2.6
1	G	121	LEU	2.6
1	D	145	GLY	2.6
1	F	145	GLY	2.6
1	S	314	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	S	16	PHE	2.6
1	L	49	ASP	2.6
1	K	5	MET	2.6
1	F	163	VAL	2.6
1	J	144	ALA	2.6
1	R	163	VAL	2.6
1	S	361	ALA	2.6
1	T	114	ALA	2.6
1	A	127	ILE	2.5
1	I	127	ILE	2.5
1	B	368	PHE	2.5
1	R	316	THR	2.5
1	E	60	ARG	2.5
1	R	274	GLY	2.5
1	K	160	GLU	2.5
1	T	74	PRO	2.5
1	T	72	VAL	2.5
1	J	127	ILE	2.5
1	A	5	MET	2.5
1	E	51	ALA	2.4
1	N	368	PHE	2.4
1	M	4	ARG	2.4
1	F	127	ILE	2.4
1	S	51	ALA	2.4
1	G	316	THR	2.4
1	R	352	THR	2.4
1	T	38	LEU	2.4
1	I	214	PRO	2.4
1	T	119	GLY	2.4
1	T	81	VAL	2.4
1	H	160	GLU	2.4
1	S	22	SER	2.4
1	M	49	ASP	2.4
1	K	50	GLY	2.4
1	L	233	GLN	2.4
1	S	4	ARG	2.4
1	F	144	ALA	2.4
1	I	86	ALA	2.4
1	A	246	TYR	2.3
1	N	55	THR	2.3
1	S	357	MET	2.3
1	I	346	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	49	ASP	2.3
1	I	4	ARG	2.3
1	M	368	PHE	2.3
1	T	30	LEU	2.3
1	T	95	ILE	2.3
1	L	246	TYR	2.3
1	O	246	TYR	2.3
1	I	216	THR	2.3
1	O	278	ASP	2.3
1	K	6	PHE	2.3
1	L	243	ALA	2.3
1	N	236	ALA	2.3
1	P	121	LEU	2.3
1	O	315	ILE	2.3
1	F	146	THR	2.3
1	N	246	TYR	2.3
1	T	146	THR	2.3
1	I	357	MET	2.3
1	S	5	MET	2.3
1	S	368	PHE	2.3
1	B	51	ALA	2.3
1	J	246	TYR	2.3
1	D	278	ASP	2.3
1	N	49	ASP	2.3
1	S	33	GLY	2.3
1	L	347	LEU	2.3
1	F	114	ALA	2.2
1	I	218	ALA	2.2
1	F	5	MET	2.2
1	R	5	MET	2.2
1	I	68	ILE	2.2
1	O	68	ILE	2.2
1	T	6	PHE	2.2
1	G	5	MET	2.2
1	I	352	THR	2.2
1	S	196	GLY	2.2
1	T	49	ASP	2.2
1	M	48	LYS	2.2
1	Q	368	PHE	2.2
1	H	216	THR	2.2
1	T	55	THR	2.2
1	T	157	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	Q	246	TYR	2.2
1	B	278	ASP	2.2
1	E	41	ASP	2.2
1	L	237	LEU	2.2
1	M	50	GLY	2.2
1	S	84	GLY	2.2
1	S	121	LEU	2.2
1	S	318	LEU	2.2
1	I	13	VAL	2.2
1	I	161	THR	2.2
1	M	246	TYR	2.2
1	F	121	LEU	2.2
1	N	71	GLY	2.2
1	K	163	VAL	2.2
1	A	19	ASN	2.1
1	R	246	TYR	2.1
1	H	121	LEU	2.1
1	H	52	VAL	2.1
1	S	239	SER	2.1
1	L	160	GLU	2.1
1	E	116	THR	2.1
1	C	121	LEU	2.1
1	J	121	LEU	2.1
1	I	145	GLY	2.1
1	A	94	ASP	2.1
1	G	315	ILE	2.1
1	N	127	ILE	2.1
1	R	315	ILE	2.1
1	G	6	PHE	2.1
1	K	368	PHE	2.1
1	R	6	PHE	2.1
1	C	144	ALA	2.1
1	I	219	ALA	2.1
1	N	352	THR	2.1
1	S	126	GLY	2.1
1	N	155	VAL	2.1
1	T	127	ILE	2.1
1	C	6	PHE	2.1
1	I	94	ASP	2.1
1	I	368	PHE	2.1
1	J	49	ASP	2.1
1	L	387	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	S	120	ASP	2.1
1	I	206	ALA	2.1
1	S	86	ALA	2.1
1	K	352	THR	2.1
1	F	315	ILE	2.1
1	L	356	TYR	2.1
1	E	82	ARG	2.0
1	I	212	ALA	2.0
1	I	316	THR	2.0
1	J	352	THR	2.0
1	N	74	PRO	2.0
1	S	68	ILE	2.0
1	O	6	PHE	2.0
1	Q	4	ARG	2.0
1	H	218	ALA	2.0
1	P	49	ASP	2.0
1	L	360	MET	2.0
1	O	143	THR	2.0
1	S	360	MET	2.0
1	G	127	ILE	2.0
1	R	374	GLY	2.0
1	G	163	VAL	2.0
1	H	215	VAL	2.0
1	H	249	TYR	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	FE2	B	1388	1/1	0.98	0.16	40,40,40,40	0
2	FE2	H	1388	1/1	0.98	0.19	31,31,31,31	0
2	FE2	J	1388	1/1	0.98	0.12	43,43,43,43	0
2	FE2	D	1388	1/1	0.99	0.18	38,38,38,38	0
2	FE2	E	1388	1/1	0.99	0.17	30,30,30,30	0
2	FE2	F	1388	1/1	0.99	0.14	51,51,51,51	0
2	FE2	G	1388	1/1	0.99	0.14	43,43,43,43	0
2	FE2	A	1388	1/1	0.99	0.15	41,41,41,41	0
2	FE2	I	1388	1/1	0.99	0.18	36,36,36,36	0
2	FE2	C	1388	1/1	0.99	0.15	43,43,43,43	0
2	FE2	K	1388	1/1	0.99	0.17	27,27,27,27	0
2	FE2	L	1388	1/1	0.99	0.17	39,39,39,39	0
2	FE2	M	1388	1/1	0.99	0.19	30,30,30,30	0
2	FE2	N	1388	1/1	0.99	0.17	44,44,44,44	0
2	FE2	P	1388	1/1	0.99	0.17	36,36,36,36	0
2	FE2	R	1388	1/1	0.99	0.14	49,49,49,49	0
2	FE2	S	1388	1/1	0.99	0.08	64,64,64,64	0
2	FE2	T	1388	1/1	0.99	0.12	65,65,65,65	0
2	FE2	Q	1388	1/1	1.00	0.19	42,42,42,42	0
2	FE2	O	1388	1/1	1.00	0.18	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.