



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:54 AM UTC

PDB ID : 5H2T / pdb_00005h2t
Title : Structure of trehalose synthase
Authors : Wang, D.; Huang, H.; Zhou, J.; Jiang, L.
Deposited on : 2016-10-18
Resolution : 2.80 Å(reported)

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

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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

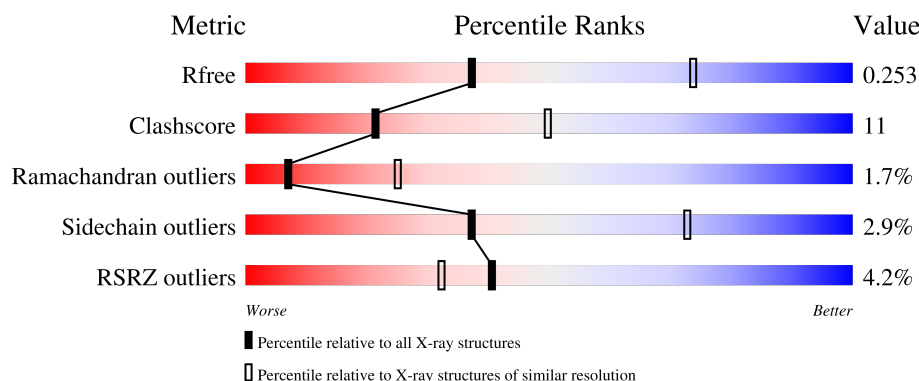
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	601	73% 17% • 9%
1	B	601	72% 17% • 9%
1	C	601	67% 21% • 9%
1	D	601	71% 17% • 9%
1	E	601	66% 22% • 9%

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Mol	Chain	Length	Quality of chain
1	F	601	9% 64% 21% • • 9%
1	G	601	2% 69% 19% • 9%
1	H	601	10% 58% 26% • • 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 35620 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.

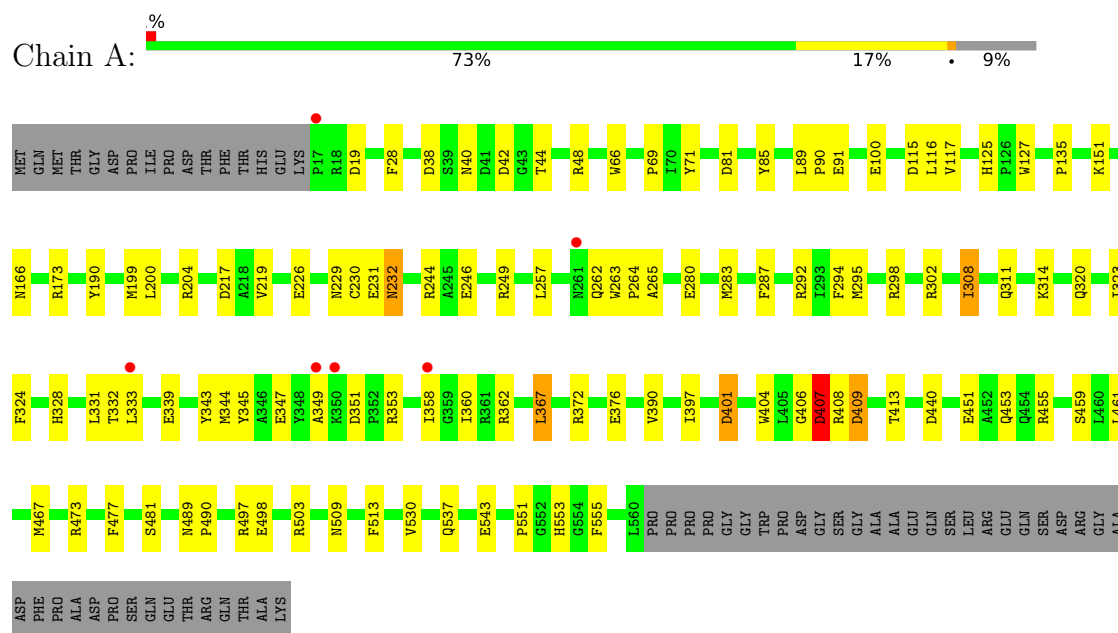
- Molecule 1 is a protein called Trehalose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	B	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	C	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	D	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	E	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	F	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	G	544	Total	C	N	O	S	0	0	0
			4462	2858	763	818	23			
1	H	536	Total	C	N	O	S	0	0	0
			4386	2810	748	805	23			

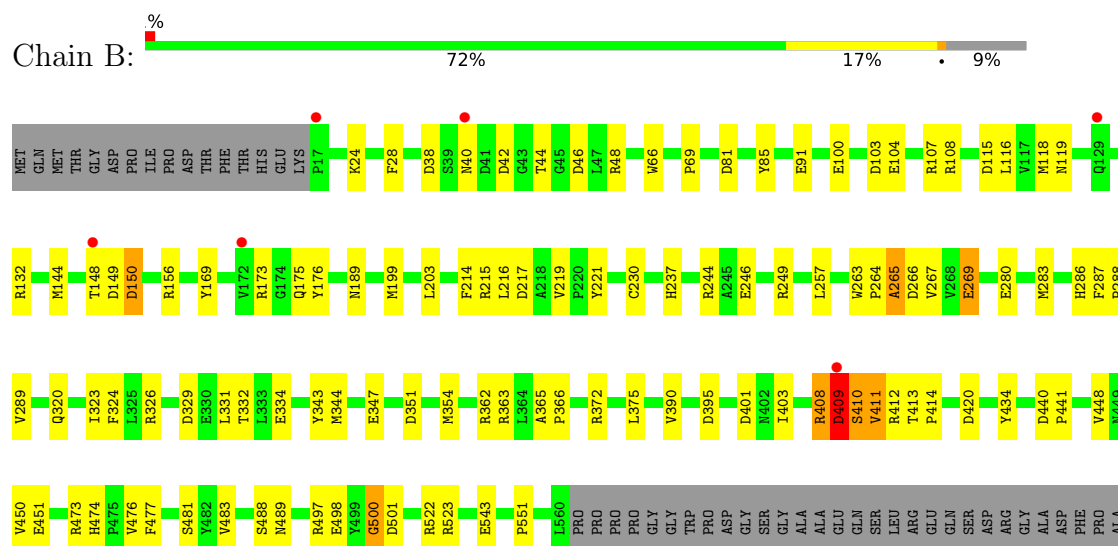
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

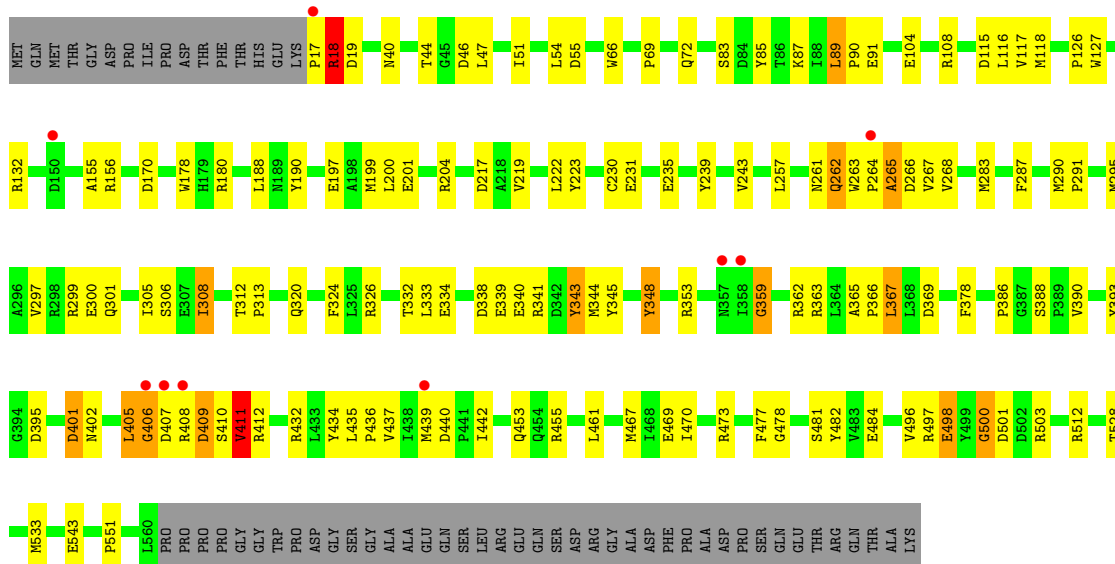
• Molecule 1: Trehalose synthase



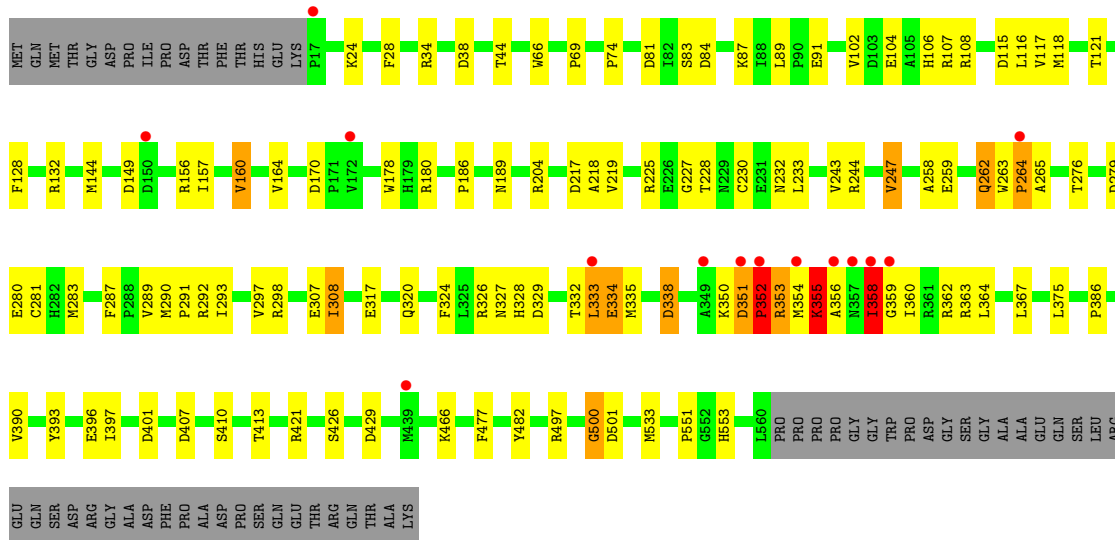
• Molecule 1: Trehalose synthase



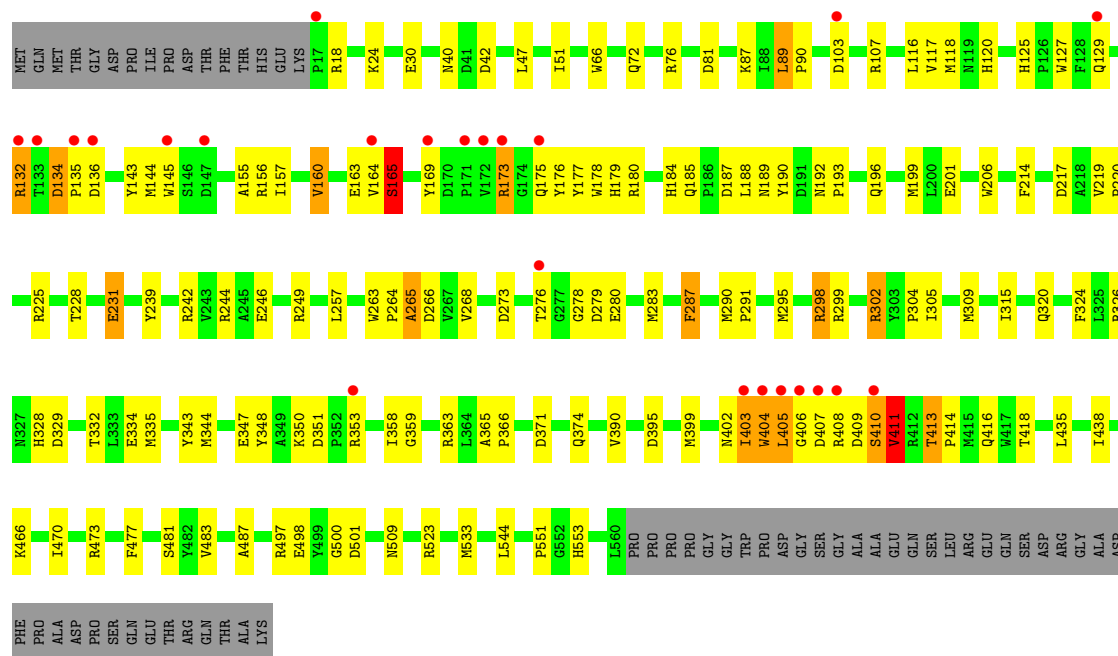
Chain C: 67% 21% 9%



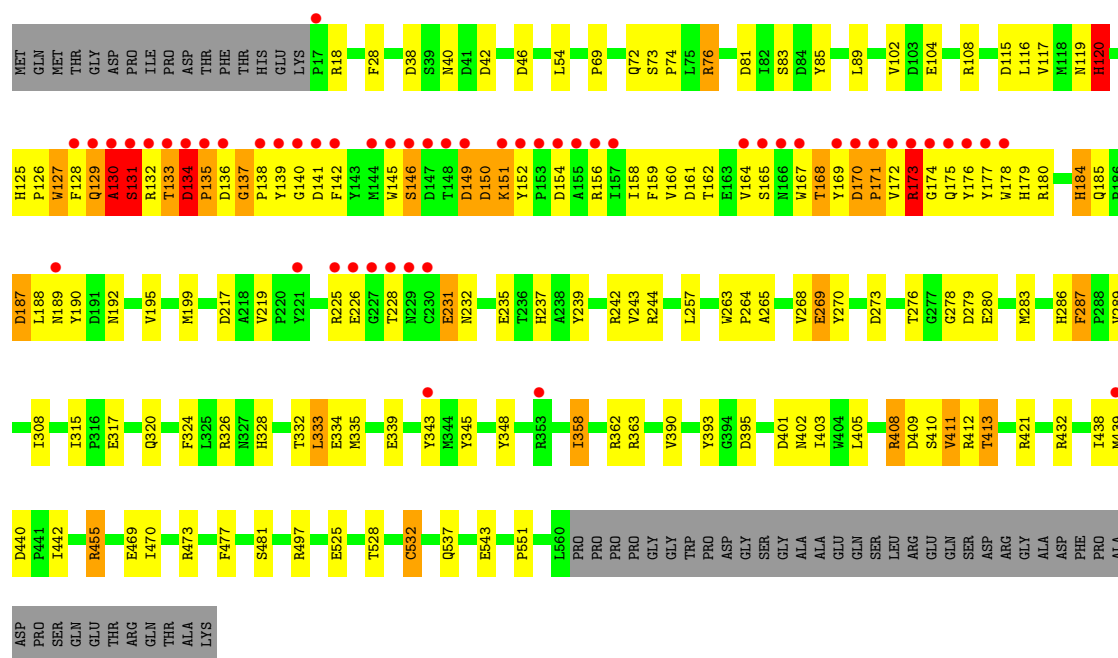
Chain D: 2% 71% 17% 9%



Chain E:



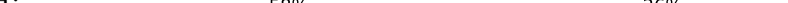
• Molecule 1: Trehalose synthase

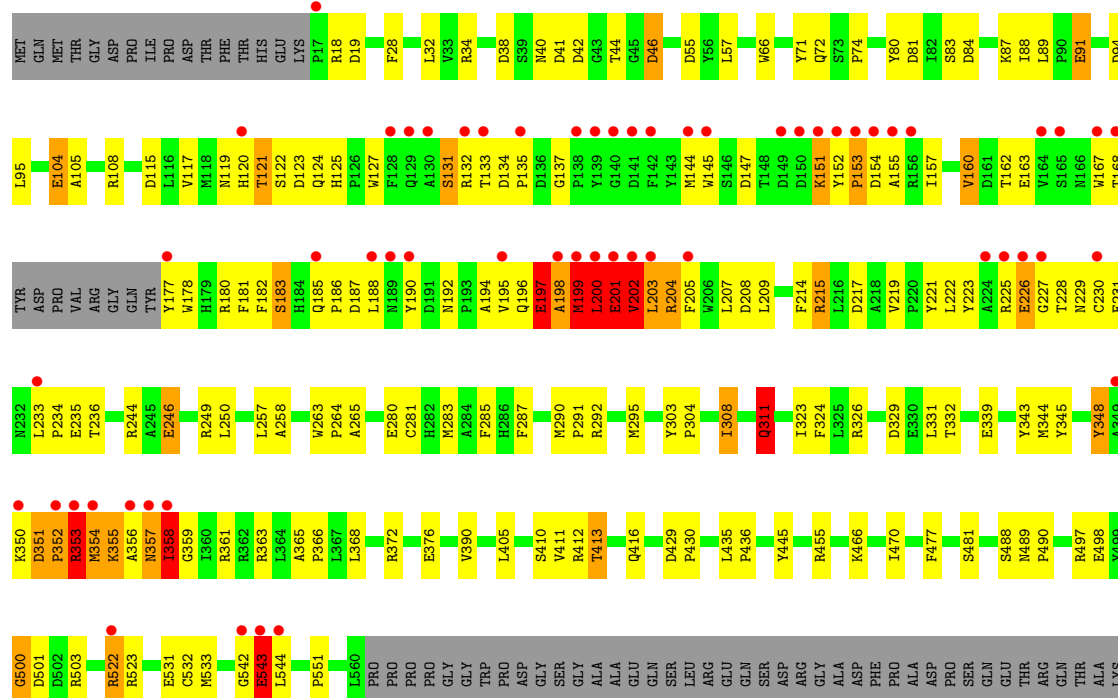


• Molecule 1: Trehalose synthase





Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.76Å 133.12Å 211.78Å 90.00° 112.54° 90.00°	Depositor
Resolution (Å)	43.57 – 2.80 43.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.57-2.80) 99.1 (43.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.205 , 0.252 0.209 , 0.253	Depositor DCC
R_{free} test set	7745 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35620	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/4599	1.01	14/6269 (0.2%)
1	B	0.82	0/4599	0.98	14/6269 (0.2%)
1	C	0.77	0/4599	0.99	18/6269 (0.3%)
1	D	0.75	0/4599	0.99	14/6269 (0.2%)
1	E	0.76	0/4599	1.00	19/6269 (0.3%)
1	F	0.79	1/4599 (0.0%)	1.08	31/6269 (0.5%)
1	G	0.73	1/4599 (0.0%)	1.00	11/6269 (0.2%)
1	H	0.78	0/4519	1.10	31/6159 (0.5%)
All	All	0.78	2/36712 (0.0%)	1.02	152/50042 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	9
All	All	0	18

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	120	HIS	CE1-NE2	6.63	1.39	1.32
1	G	404	TRP	CD2-CE2	5.07	1.50	1.41

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	199	MET	N-CA-C	-10.79	100.35	113.19
1	B	408	ARG	N-CA-C	-9.89	96.70	110.35
1	F	408	ARG	N-CA-C	-9.18	96.19	110.42
1	C	287	PHE	CA-C-N	-9.06	110.39	120.45
1	C	287	PHE	C-N-CA	-9.06	110.39	120.45
1	H	133	THR	N-CA-C	-9.01	100.61	111.69
1	G	219	VAL	CA-C-N	-8.84	111.16	119.82
1	G	219	VAL	C-N-CA	-8.84	111.16	119.82
1	H	358	ILE	N-CA-C	-8.78	101.66	110.62
1	A	332	THR	CA-C-N	-8.54	111.35	122.79
1	A	332	THR	C-N-CA	-8.54	111.35	122.79
1	H	543	GLU	N-CA-C	8.50	123.86	107.71
1	A	332	THR	N-CA-C	-8.39	96.25	109.50
1	F	152	TYR	CA-C-N	8.37	129.37	120.83
1	F	152	TYR	C-N-CA	8.37	129.37	120.83
1	H	201	GLU	N-CA-C	-8.36	92.99	110.80
1	H	542	GLY	N-CA-C	-8.32	100.71	112.60
1	B	332	THR	CA-C-N	-8.22	111.77	122.79
1	B	332	THR	C-N-CA	-8.22	111.77	122.79
1	F	168	THR	N-CA-C	8.21	119.40	108.07
1	E	219	VAL	CA-C-N	-8.13	111.85	119.82
1	E	219	VAL	C-N-CA	-8.13	111.85	119.82
1	F	219	VAL	CA-C-N	-8.05	111.50	119.87
1	F	219	VAL	C-N-CA	-8.05	111.50	119.87
1	B	411	VAL	N-CA-C	-7.86	104.70	112.17
1	B	332	THR	N-CA-C	-7.78	97.56	109.85
1	H	227	GLY	N-CA-C	-7.59	102.41	115.61
1	B	287	PHE	CA-C-N	-7.58	112.04	120.45
1	B	287	PHE	C-N-CA	-7.58	112.04	120.45
1	C	219	VAL	CA-C-N	-7.55	112.42	119.82
1	C	219	VAL	C-N-CA	-7.55	112.42	119.82
1	G	262	GLN	N-CA-C	7.44	120.72	109.41
1	D	219	VAL	CA-C-N	-7.42	112.16	119.87
1	D	219	VAL	C-N-CA	-7.42	112.16	119.87
1	H	152	TYR	CA-C-N	7.41	129.10	119.84
1	H	152	TYR	C-N-CA	7.41	129.10	119.84
1	H	357	ASN	N-CA-C	-7.34	101.40	110.65
1	D	355	LYS	N-CA-C	-7.31	97.68	109.96
1	H	311	GLN	CA-CB-CG	7.23	128.57	114.10
1	A	287	PHE	CA-C-N	-7.21	112.12	120.12
1	A	287	PHE	C-N-CA	-7.21	112.12	120.12
1	G	404	TRP	CG-CD2-CE3	7.13	141.03	133.90
1	F	164	VAL	N-CA-C	-7.08	102.37	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	200	LEU	CA-CB-CG	6.99	140.76	116.30
1	G	474	HIS	N-CA-CB	-6.95	102.47	111.09
1	B	409	ASP	N-CA-C	-6.88	96.14	110.80
1	B	219	VAL	CA-C-N	-6.87	113.09	119.82
1	B	219	VAL	C-N-CA	-6.87	113.09	119.82
1	E	134	ASP	CA-C-N	6.86	126.56	119.56
1	E	134	ASP	C-N-CA	6.86	126.56	119.56
1	H	219	VAL	CA-C-N	-6.62	112.99	119.87
1	H	219	VAL	C-N-CA	-6.62	112.99	119.87
1	D	353	ARG	N-CA-C	-6.61	104.47	112.54
1	E	165	SER	N-CA-C	6.56	118.48	110.41
1	G	149	ASP	N-CA-C	6.37	120.75	112.92
1	F	174	GLY	N-CA-C	6.30	124.79	115.08
1	B	266	ASP	N-CA-C	-6.29	105.09	112.89
1	D	265	ALA	N-CA-C	-6.24	104.41	114.09
1	F	411	VAL	N-CA-C	-6.19	96.47	109.34
1	F	173	ARG	CB-CG-CD	6.16	125.48	111.30
1	F	154	ASP	N-CA-C	-6.15	105.71	112.72
1	H	197	GLU	CA-CB-CG	6.14	126.39	114.10
1	E	411	VAL	N-CA-C	-6.13	96.58	109.34
1	H	353	ARG	N-CA-C	-6.11	103.94	112.25
1	H	200	LEU	N-CA-C	-6.07	97.88	110.80
1	G	333	LEU	CA-CB-CG	6.06	137.52	116.30
1	C	18	ARG	N-CA-C	6.03	118.55	111.02
1	E	89	LEU	CA-C-N	6.00	126.43	119.47
1	E	89	LEU	C-N-CA	6.00	126.43	119.47
1	G	266	ASP	N-CA-C	-5.96	105.50	112.89
1	C	359	GLY	N-CA-C	-5.91	99.17	113.18
1	H	348	TYR	N-CA-C	-5.91	105.33	112.54
1	E	287	PHE	CA-C-N	-5.91	113.56	120.12
1	E	287	PHE	C-N-CA	-5.91	113.56	120.12
1	A	226	GLU	N-CA-C	-5.87	101.15	109.96
1	H	287	PHE	CA-C-N	-5.84	113.63	120.12
1	H	287	PHE	C-N-CA	-5.84	113.63	120.12
1	C	19	ASP	CA-C-N	5.84	125.46	119.56
1	C	19	ASP	C-N-CA	5.84	125.46	119.56
1	F	134	ASP	CA-C-N	-5.80	112.59	119.84
1	F	134	ASP	C-N-CA	-5.80	112.59	119.84
1	F	119	ASN	CA-C-N	-5.74	111.81	121.75
1	F	119	ASN	C-N-CA	-5.74	111.81	121.75
1	E	266	ASP	N-CA-C	-5.74	105.78	112.89
1	A	232	ASN	N-CA-CB	-5.73	103.53	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	149	ASP	CA-C-N	-5.71	114.04	122.83
1	G	149	ASP	C-N-CA	-5.71	114.04	122.83
1	H	155	ALA	N-CA-C	-5.68	99.92	108.96
1	C	89	LEU	CA-C-N	5.68	126.06	119.47
1	C	89	LEU	C-N-CA	5.68	126.06	119.47
1	A	219	VAL	CA-C-N	-5.68	114.26	119.82
1	A	219	VAL	C-N-CA	-5.68	114.26	119.82
1	H	202	VAL	O-C-N	5.65	127.59	121.94
1	A	543	GLU	N-CA-C	-5.59	106.50	113.38
1	C	411	VAL	N-CA-CB	-5.58	104.85	112.28
1	F	287	PHE	CA-C-N	-5.58	113.92	120.12
1	F	287	PHE	C-N-CA	-5.58	113.92	120.12
1	A	19	ASP	CA-C-N	5.57	125.10	119.19
1	A	19	ASP	C-N-CA	5.57	125.10	119.19
1	F	532	CYS	N-CA-C	5.48	117.34	111.36
1	G	180	ARG	N-CA-C	-5.46	106.62	113.28
1	H	413	THR	CA-C-N	5.43	125.44	119.90
1	H	413	THR	C-N-CA	5.43	125.44	119.90
1	F	146	SER	N-CA-C	5.42	118.02	108.75
1	D	89	LEU	CA-C-N	5.38	125.20	119.28
1	D	89	LEU	C-N-CA	5.38	125.20	119.28
1	E	132	ARG	N-CA-C	5.36	121.23	114.31
1	E	189	ASN	CA-C-N	-5.34	112.70	122.38
1	E	189	ASN	C-N-CA	-5.34	112.70	122.38
1	C	528	THR	CB-CA-C	5.34	115.78	110.33
1	D	332	THR	N-CA-C	-5.33	105.61	113.61
1	H	41	ASP	N-CA-C	5.33	119.08	112.58
1	E	353	ARG	CA-C-N	5.32	127.41	120.28
1	E	353	ARG	C-N-CA	5.32	127.41	120.28
1	B	489	ASN	CA-C-N	5.31	125.39	119.87
1	B	489	ASN	C-N-CA	5.31	125.39	119.87
1	F	137	GLY	CA-C-N	5.28	139.68	127.00
1	F	137	GLY	C-N-CA	5.28	139.68	127.00
1	B	132	ARG	N-CA-C	-5.27	107.40	113.88
1	F	137	GLY	C-N-CD	-5.25	109.05	120.60
1	F	130	ALA	N-CA-C	-5.24	99.63	110.80
1	F	185	GLN	CA-C-N	5.23	124.99	119.76
1	F	185	GLN	C-N-CA	5.23	124.99	119.76
1	C	348	TYR	N-CA-C	-5.22	105.71	111.71
1	F	403	ILE	CB-CA-C	-5.21	104.44	112.05
1	H	204	ARG	CB-CA-C	-5.21	102.94	110.96
1	C	388	SER	CA-C-N	5.20	125.65	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	SER	C-N-CA	5.20	125.65	120.14
1	H	356	ALA	N-CA-C	-5.18	107.12	112.93
1	F	162	THR	N-CA-C	-5.16	107.64	114.04
1	F	358	ILE	N-CA-C	5.15	115.92	110.72
1	H	19	ASP	CA-C-N	5.14	124.75	119.56
1	H	19	ASP	C-N-CA	5.14	124.75	119.56
1	E	164	VAL	N-CA-C	-5.14	105.36	112.50
1	F	184	HIS	N-CA-C	-5.12	106.88	113.02
1	D	333	LEU	N-CA-C	-5.10	99.45	108.08
1	F	170	ASP	CA-C-N	-5.10	113.47	119.84
1	F	170	ASP	C-N-CA	-5.10	113.47	119.84
1	H	105	ALA	N-CA-C	-5.10	105.62	111.07
1	D	227	GLY	N-CA-C	-5.09	107.96	114.37
1	H	202	VAL	CA-C-O	5.09	126.56	121.27
1	C	543	GLU	N-CA-C	-5.08	107.13	113.38
1	C	18	ARG	CA-C-N	-5.07	117.37	122.74
1	C	18	ARG	C-N-CA	-5.07	117.37	122.74
1	E	418	THR	CA-C-N	-5.07	113.51	119.84
1	E	418	THR	C-N-CA	-5.07	113.51	119.84
1	D	358	ILE	CA-C-N	5.03	130.75	121.70
1	D	358	ILE	C-N-CA	5.03	130.75	121.70
1	A	229	ASN	N-CA-C	-5.02	107.20	113.38
1	D	352	PRO	CA-C-N	5.02	129.10	120.72
1	D	352	PRO	C-N-CA	5.02	129.10	120.72
1	A	166	ASN	N-CA-C	-5.01	106.86	113.17

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	D	351	ASP	Peptide
1	D	352	PRO	Peptide
1	E	165	SER	Peptide
1	E	410	SER	Peptide
1	F	131	SER	Peptide
1	F	149	ASP	Peptide
1	G	225	ARG	Peptide
1	G	333	LEU	Peptide
1	H	131	SER	Peptide
1	H	196	GLN	Peptide
1	H	199	MET	Peptide

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Mol	Chain	Res	Type	Group
1	H	200	LEU	Peptide
1	H	202	VAL	Peptide
1	H	350	LYS	Peptide
1	H	352	PRO	Peptide
1	H	353	ARG	Peptide
1	H	543	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4462	0	4252	63	0
1	B	4462	0	4252	71	0
1	C	4462	0	4252	90	0
1	D	4462	0	4252	83	0
1	E	4462	0	4252	106	0
1	F	4462	0	4252	121	0
1	G	4462	0	4252	88	0
1	H	4386	0	4178	151	0
All	All	35620	0	33942	759	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 11.

All (759) 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:D:356:ALA:HB1	1:D:360:ILE:H	0.99	1.13
1:D:334:GLU:N	1:D:358:ILE:O	1.99	0.94
1:D:356:ALA:HB1	1:D:360:ILE:N	1.83	0.94
1:H:201:GLU:O	1:H:204:ARG:N	2.04	0.91
1:A:125:HIS:HD2	1:A:127:TRP:H	1.20	0.90
1:F:133:THR:HG23	1:F:134:ASP:HA	1.54	0.90
1:H:188:LEU:HD13	1:H:199:MET:HE3	1.52	0.88
1:D:352:PRO:HA	1:D:354:MET:HG2	1.56	0.87
1:E:196:GLN:OE1	1:E:242:ARG:NH1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:LEU:HB3	1:D:359:GLY:H	1.40	0.85
1:G:332:THR:HG23	1:G:334:GLU:H	1.38	0.85
1:D:477:PHE:O	1:D:497:ARG:NH2	2.10	0.85
1:F:137:GLY:N	1:F:139:TYR:H	1.76	0.84
1:E:407:ASP:OD1	1:E:410:SER:N	2.09	0.83
1:A:232:ASN:ND2	1:A:262:GLN:HE22	1.76	0.83
1:B:119:ASN:HD21	1:B:221:TYR:HB2	1.43	0.82
1:H:197:GLU:O	1:H:200:LEU:N	2.09	0.82
1:F:137:GLY:H	1:F:139:TYR:H	1.28	0.82
1:G:477:PHE:O	1:G:497:ARG:NH2	2.12	0.82
1:C:551:PRO:HG3	1:E:551:PRO:HG3	1.61	0.82
1:C:72:GLN:HG3	1:C:87:LYS:HD3	1.62	0.81
1:B:119:ASN:ND2	1:B:221:TYR:HB2	1.94	0.81
1:A:372:ARG:NH1	1:A:376:GLU:OE2	2.13	0.81
1:F:170:ASP:HB2	1:F:173:ARG:HG3	1.63	0.80
1:F:332:THR:O	1:F:334:GLU:N	2.15	0.80
1:C:156:ARG:O	1:C:180:ARG:NH1	2.15	0.80
1:H:355:LYS:N	1:H:357:ASN:OD1	2.14	0.80
1:E:477:PHE:O	1:E:497:ARG:NH2	2.15	0.79
1:H:226:GLU:H	1:H:228:THR:H	1.28	0.78
1:B:551:PRO:HG3	1:D:551:PRO:HG3	1.66	0.77
1:F:117:VAL:HG11	1:F:120:HIS:CE1	2.19	0.77
1:H:522:ARG:HH22	1:H:544:LEU:HA	1.50	0.77
1:H:225:ARG:HG2	1:H:233:LEU:HD13	1.66	0.76
1:C:477:PHE:O	1:C:497:ARG:NH2	2.18	0.76
1:F:131:SER:HB3	1:F:173:ARG:HB3	1.67	0.76
1:B:363:ARG:HG3	1:B:395:ASP:OD1	1.86	0.76
1:F:551:PRO:HG3	1:G:551:PRO:HG3	1.68	0.76
1:H:200:LEU:O	1:H:201:GLU:HG3	1.87	0.75
1:B:477:PHE:O	1:B:497:ARG:NH2	2.19	0.75
1:F:165:SER:OG	1:F:167:TRP:O	2.05	0.75
1:F:363:ARG:HG2	1:F:395:ASP:OD1	1.87	0.74
1:E:399:MET:HE3	1:E:416:GLN:HE21	1.51	0.74
1:F:455:ARG:HG3	1:F:455:ARG:HH11	1.51	0.74
1:A:498:GLU:OE2	1:A:503:ARG:NH1	2.20	0.73
1:A:246:GLU:OE2	1:A:249:ARG:NH1	2.22	0.73
1:G:244:ARG:HD3	1:G:280:GLU:O	1.88	0.73
1:E:470:ILE:HD13	1:E:473:ARG:HH21	1.54	0.73
1:C:295:MET:HE3	1:C:348:TYR:HD1	1.54	0.72
1:C:406:GLY:O	1:C:407:ASP:HB3	1.89	0.72
1:F:170:ASP:OD1	1:F:170:ASP:N	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:ASP:O	1:F:410:SER:OG	2.06	0.72
1:C:408:ARG:O	1:C:409:ASP:HB2	1.89	0.71
1:G:226:GLU:O	1:G:228:THR:HG23	1.90	0.71
1:H:351:ASP:HB3	1:H:352:PRO:HA	1.72	0.71
1:H:498:GLU:OE2	1:H:523:ARG:NH2	2.23	0.71
1:C:332:THR:O	1:C:334:GLU:N	2.23	0.71
1:A:477:PHE:O	1:A:497:ARG:NH2	2.24	0.71
1:E:188:LEU:HD13	1:E:199:MET:HE3	1.73	0.70
1:F:477:PHE:O	1:F:497:ARG:NH2	2.24	0.70
1:G:55:ASP:OD1	1:G:108:ARG:NH2	2.22	0.70
1:F:283:MET:HG2	1:F:320:GLN:HB3	1.72	0.70
1:F:156:ARG:O	1:F:180:ARG:NH1	2.24	0.70
1:B:409:ASP:O	1:B:411:VAL:N	2.21	0.70
1:D:356:ALA:CB	1:D:360:ILE:H	1.93	0.69
1:H:194:ALA:C	1:H:197:GLU:HB3	2.16	0.69
1:C:362:ARG:HB2	1:C:367:LEU:HD13	1.73	0.69
1:E:72:GLN:HG3	1:E:87:LYS:HD3	1.75	0.69
1:H:198:ALA:C	1:H:200:LEU:N	2.50	0.69
1:E:184:HIS:HD2	1:E:185:GLN:HG3	1.58	0.69
1:F:40:ASN:ND2	1:F:42:ASP:OD1	2.26	0.69
1:A:551:PRO:HG3	1:H:551:PRO:HG3	1.74	0.69
1:G:328:HIS:NE2	1:G:358:ILE:O	2.25	0.69
1:A:406:GLY:O	1:A:408:ARG:N	2.25	0.68
1:E:156:ARG:O	1:E:180:ARG:NH1	2.27	0.68
1:C:467:MET:HE2	1:C:533:MET:SD	2.34	0.68
1:G:232:ASN:OD1	1:G:262:GLN:NE2	2.27	0.68
1:H:188:LEU:CD1	1:H:199:MET:HE3	2.24	0.68
1:H:40:ASN:ND2	1:H:46:ASP:OD1	2.27	0.68
1:D:232:ASN:ND2	1:D:262:GLN:OE1	2.27	0.68
1:E:407:ASP:OD1	1:E:409:ASP:N	2.27	0.67
1:F:276:THR:HG23	1:F:278:GLY:H	1.59	0.67
1:D:334:GLU:H	1:D:358:ILE:C	2.02	0.67
1:C:353:ARG:NH1	1:C:369:ASP:OD2	2.28	0.67
1:H:372:ARG:NH1	1:H:376:GLU:OE2	2.27	0.67
1:C:363:ARG:HG2	1:C:395:ASP:OD1	1.94	0.67
1:H:200:LEU:HB3	1:H:202:VAL:N	2.10	0.67
1:E:405:LEU:HD23	1:E:435:LEU:HD22	1.77	0.67
1:F:128:PHE:O	1:F:130:ALA:N	2.28	0.66
1:F:104:GLU:OE1	1:F:108:ARG:NH1	2.27	0.66
1:G:188:LEU:HD13	1:G:199:MET:HE3	1.77	0.66
1:E:145:TRP:CH2	1:E:173:ARG:HD3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:ASN:O	1:H:231:GLU:N	2.29	0.66
1:F:130:ALA:HA	1:F:132:ARG:H	1.58	0.66
1:H:83:SER:O	1:H:125:HIS:ND1	2.25	0.66
1:H:120:HIS:CD2	1:H:185:GLN:HB3	2.30	0.66
1:H:498:GLU:HG2	1:H:503:ARG:HG2	1.78	0.66
1:G:473:ARG:O	1:G:474:HIS:HD2	1.79	0.66
1:C:132:ARG:HD2	1:C:170:ASP:OD2	1.95	0.66
1:H:470:ILE:HD13	1:H:532:CYS:HB3	1.78	0.66
1:C:266:ASP:OD1	1:C:341:ARG:NH1	2.27	0.65
1:F:72:GLN:HA	1:F:89:LEU:HD13	1.77	0.65
1:E:295:MET:SD	1:E:298:ARG:NH1	2.69	0.65
1:H:500:GLY:O	1:H:501:ASP:HB2	1.96	0.65
1:H:257:LEU:HG	1:H:283:MET:HB2	1.77	0.65
1:B:498:GLU:OE2	1:B:523:ARG:NH1	2.30	0.65
1:C:409:ASP:HA	1:C:412:ARG:HB2	1.79	0.65
1:E:332:THR:O	1:E:334:GLU:N	2.30	0.65
1:D:354:MET:HG3	1:D:355:LYS:N	2.12	0.65
1:F:180:ARG:NH2	1:F:231:GLU:OE1	2.29	0.65
1:G:287:PHE:CE1	1:G:329:ASP:HB3	2.32	0.65
1:G:320:GLN:NE2	1:G:478:GLY:O	2.28	0.65
1:D:156:ARG:O	1:D:180:ARG:NH1	2.30	0.64
1:A:44:THR:HG21	1:A:91:GLU:HG2	1.78	0.64
1:E:276:THR:HG21	1:E:279:ASP:HB3	1.78	0.64
1:H:95:LEU:HD23	1:H:205:PHE:HZ	1.61	0.64
1:H:522:ARG:HH12	1:H:544:LEU:C	2.06	0.64
1:B:118:MET:HE3	1:B:216:LEU:HD22	1.79	0.64
1:B:40:ASN:ND2	1:B:42:ASP:OD1	2.31	0.64
1:D:354:MET:HG3	1:D:355:LYS:HG3	1.79	0.64
1:D:355:LYS:HD2	1:D:362:ARG:HG3	1.80	0.64
1:G:237:HIS:CE1	1:G:269:GLU:HG2	2.33	0.64
1:H:203:LEU:HD12	1:H:203:LEU:H	1.63	0.64
1:E:163:GLU:HG3	1:E:165:SER:HB3	1.79	0.64
1:F:363:ARG:NH1	1:F:393:TYR:O	2.31	0.63
1:C:104:GLU:OE1	1:C:108:ARG:NH1	2.31	0.63
1:H:95:LEU:HD23	1:H:205:PHE:CZ	2.34	0.63
1:B:522:ARG:HD3	1:B:543:GLU:HG3	1.80	0.63
1:B:116:LEU:HD23	1:B:118:MET:HE2	1.79	0.63
1:E:295:MET:SD	1:E:298:ARG:NH2	2.72	0.63
1:E:283:MET:HG2	1:E:320:GLN:HB3	1.79	0.63
1:H:74:PRO:HD3	1:H:83:SER:OG	1.98	0.63
1:E:276:THR:HG23	1:E:278:GLY:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:ASP:C	1:E:409:ASP:H	2.04	0.63
1:F:273:ASP:O	1:F:276:THR:HG22	1.99	0.63
1:H:354:MET:HG3	1:H:357:ASN:OD1	1.98	0.62
1:H:477:PHE:O	1:H:497:ARG:NH2	2.33	0.62
1:H:134:ASP:HB3	1:H:137:GLY:HA3	1.82	0.62
1:D:132:ARG:HD2	1:D:170:ASP:OD2	1.99	0.62
1:D:351:ASP:C	1:D:353:ARG:H	2.07	0.62
1:B:173:ARG:NE	1:B:175:GLN:OE1	2.31	0.62
1:F:339:GLU:HG2	1:F:345:TYR:CZ	2.34	0.62
1:C:295:MET:HE3	1:C:348:TYR:CD1	2.35	0.62
1:H:522:ARG:HH22	1:H:544:LEU:CA	2.12	0.62
1:F:131:SER:CB	1:F:173:ARG:HB3	2.29	0.62
1:G:156:ARG:O	1:G:180:ARG:NH2	2.29	0.62
1:C:116:LEU:HD22	1:C:118:MET:HE3	1.82	0.61
1:A:360:ILE:HA	1:A:407:ASP:HB2	1.82	0.61
1:C:407:ASP:O	1:C:408:ARG:HG2	2.01	0.61
1:F:125:HIS:HD1	1:F:126:PRO:HD2	1.65	0.61
1:F:232:ASN:OD1	1:F:270:TYR:OH	2.11	0.61
1:A:343:TYR:CE2	1:A:344:MET:HE3	2.36	0.61
1:F:328:HIS:NE2	1:F:358:ILE:O	2.33	0.61
1:G:263:TRP:CD2	1:G:264:PRO:HD2	2.35	0.61
1:H:127:TRP:HZ3	1:H:199:MET:HE1	1.65	0.61
1:D:28:PHE:HB2	1:D:390:VAL:HG22	1.83	0.61
1:E:145:TRP:HB3	1:E:175:GLN:NE2	2.15	0.61
1:E:328:HIS:NE2	1:E:358:ILE:O	2.33	0.61
1:H:225:ARG:O	1:H:228:THR:OG1	2.17	0.61
1:E:403:ILE:O	1:E:405:LEU:N	2.30	0.61
1:F:130:ALA:HA	1:F:132:ARG:N	2.15	0.61
1:B:343:TYR:CE2	1:B:344:MET:HE3	2.35	0.61
1:A:257:LEU:HG	1:A:283:MET:HB2	1.82	0.60
1:H:190:TYR:HA	1:H:195:VAL:HG21	1.83	0.60
1:F:117:VAL:HA	1:F:217:ASP:HB2	1.81	0.60
1:F:192:ASN:O	1:F:195:VAL:HG22	2.00	0.60
1:E:295:MET:SD	1:E:298:ARG:CZ	2.90	0.60
1:A:190:TYR:OH	1:A:199:MET:HG3	2.01	0.60
1:C:55:ASP:OD1	1:C:108:ARG:NH2	2.29	0.60
1:D:355:LYS:HE3	1:D:367:LEU:HD23	1.83	0.60
1:E:134:ASP:HB2	1:E:136:ASP:OD1	2.02	0.60
1:H:339:GLU:HG3	1:H:345:TYR:CD2	2.36	0.60
1:F:40:ASN:OD1	1:F:40:ASN:N	2.34	0.60
1:C:434:TYR:O	1:C:435:LEU:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:MET:HG3	1:D:355:LYS:H	1.67	0.60
1:G:333:LEU:HD13	1:G:334:GLU:HG3	1.84	0.60
1:A:231:GLU:HB3	1:A:232:ASN:HD22	1.66	0.60
1:H:84:ASP:CG	1:H:87:LYS:HD3	2.27	0.60
1:B:286:HIS:O	1:B:289:VAL:HG12	2.01	0.59
1:E:363:ARG:HG2	1:E:395:ASP:OD1	2.01	0.59
1:E:135:PRO:HB3	1:E:173:ARG:HH12	1.66	0.59
1:A:283:MET:HG2	1:A:320:GLN:HB3	1.84	0.59
1:D:283:MET:HG2	1:D:320:GLN:HB3	1.85	0.59
1:F:408:ARG:O	1:F:409:ASP:HB2	2.03	0.59
1:G:244:ARG:NH1	1:G:248:ASP:OD2	2.36	0.59
1:H:343:TYR:CE2	1:H:344:MET:HE2	2.38	0.59
1:D:328:HIS:CE1	1:D:356:ALA:HB3	2.38	0.58
1:D:66:TRP:CD1	1:D:66:TRP:C	2.81	0.58
1:D:421:ARG:NH1	1:G:451:GLU:OE2	2.22	0.58
1:E:116:LEU:HD22	1:E:118:MET:HE2	1.84	0.58
1:G:470:ILE:HD13	1:G:532:CYS:HB3	1.85	0.58
1:H:83:SER:C	1:H:125:HIS:HD1	2.10	0.58
1:H:151:LYS:NZ	1:H:226:GLU:OE1	2.36	0.58
1:G:329:ASP:OD1	1:G:332:THR:HG22	2.04	0.58
1:B:169:TYR:HB2	1:B:176:TYR:CE1	2.38	0.58
1:D:24:LYS:NZ	1:D:317:GLU:O	2.26	0.58
1:E:225:ARG:O	1:E:228:THR:HG22	2.04	0.58
1:F:362:ARG:HD2	1:F:401:ASP:OD2	2.04	0.58
1:B:362:ARG:CZ	1:B:403:ILE:HD11	2.32	0.58
1:C:261:ASN:ND2	1:C:261:ASN:O	2.37	0.58
1:F:76:ARG:HD3	1:F:184:HIS:CD2	2.38	0.58
1:D:333:LEU:HB3	1:D:359:GLY:N	2.15	0.58
1:E:298:ARG:NH2	1:E:351:ASP:HB2	2.18	0.58
1:G:72:GLN:HG3	1:G:83:SER:HB2	1.85	0.58
1:A:232:ASN:HD21	1:A:262:GLN:HE22	1.49	0.58
1:G:257:LEU:HG	1:G:283:MET:HB2	1.86	0.58
1:H:292:ARG:NH1	1:H:308:ILE:HG23	2.19	0.57
1:C:85:TYR:CE2	1:C:199:MET:HE1	2.39	0.57
1:B:148:THR:OG1	1:B:150:ASP:OD2	2.18	0.57
1:C:339:GLU:HG2	1:C:345:TYR:CE2	2.39	0.57
1:H:326:ARG:HB2	1:H:361:ARG:NH1	2.19	0.57
1:B:409:ASP:C	1:B:411:VAL:H	2.11	0.57
1:F:150:ASP:OD1	1:F:151:LYS:N	2.28	0.57
1:G:127:TRP:HZ3	1:G:199:MET:HE2	1.69	0.57
1:G:344:MET:HE2	1:G:347:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:473:ARG:O	1:G:474:HIS:CD2	2.58	0.57
1:B:451:GLU:OE2	1:F:421:ARG:NH1	2.31	0.57
1:C:500:GLY:O	1:C:501:ASP:HB2	2.05	0.57
1:H:203:LEU:O	1:H:207:LEU:HB2	2.05	0.57
1:H:263:TRP:CD2	1:H:264:PRO:HD2	2.38	0.57
1:A:125:HIS:CD2	1:A:127:TRP:H	2.11	0.57
1:B:103:ASP:HB3	1:B:107:ARG:NH1	2.19	0.57
1:B:257:LEU:HG	1:B:283:MET:HB2	1.86	0.57
1:E:145:TRP:HB3	1:E:175:GLN:HE21	1.69	0.57
1:G:498:GLU:OE2	1:G:523:ARG:NH2	2.38	0.57
1:D:74:PRO:HD3	1:D:83:SER:OG	2.04	0.57
1:E:302:ARG:NH2	1:E:487:ALA:O	2.37	0.56
1:E:324:PHE:CD1	1:E:326:ARG:HG2	2.40	0.56
1:F:244:ARG:HD2	1:F:280:GLU:O	2.05	0.56
1:A:408:ARG:O	1:A:409:ASP:HB2	2.04	0.56
1:B:263:TRP:CD2	1:B:264:PRO:HD2	2.40	0.56
1:E:129:GLN:OE1	1:E:132:ARG:NE	2.36	0.56
1:G:363:ARG:HG2	1:G:395:ASP:OD1	2.05	0.56
1:H:38:ASP:OD1	1:H:40:ASN:ND2	2.38	0.56
1:H:246:GLU:OE2	1:H:249:ARG:NH2	2.27	0.56
1:G:225:ARG:HE	1:G:235:GLU:HG2	1.70	0.56
1:H:201:GLU:O	1:H:204:ARG:HG3	2.05	0.56
1:F:168:THR:HG23	1:F:179:HIS:NE2	2.20	0.56
1:G:362:ARG:HB2	1:G:367:LEU:HD13	1.87	0.56
1:F:257:LEU:HG	1:F:283:MET:HB2	1.88	0.56
1:G:261:ASN:C	1:G:262:GLN:HG2	2.30	0.56
1:H:87:LYS:HD2	1:H:87:LYS:N	2.20	0.56
1:D:364:LEU:HG	1:D:375:LEU:HD23	1.86	0.56
1:D:500:GLY:O	1:D:501:ASP:HB2	2.05	0.56
1:F:263:TRP:CD2	1:F:264:PRO:HD2	2.41	0.56
1:A:292:ARG:HG3	1:A:308:ILE:HG12	1.88	0.56
1:C:320:GLN:NE2	1:C:478:GLY:O	2.35	0.56
1:E:402:ASN:ND2	1:E:405:LEU:HD11	2.20	0.56
1:A:44:THR:HG21	1:A:91:GLU:CG	2.36	0.55
1:F:409:ASP:HA	1:F:412:ARG:HB2	1.88	0.55
1:H:119:ASN:ND2	1:H:187:ASP:OD1	2.39	0.55
1:H:104:GLU:CD	1:H:108:ARG:HH12	2.14	0.55
1:C:469:GLU:OE2	1:C:473:ARG:NH1	2.39	0.55
1:F:170:ASP:HB2	1:F:173:ARG:CG	2.36	0.55
1:F:402:ASN:O	1:F:410:SER:HB2	2.06	0.55
1:G:232:ASN:CG	1:G:262:GLN:HE22	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:329:ASP:OD1	1:H:332:THR:OG1	2.20	0.55
1:D:225:ARG:O	1:D:228:THR:HG22	2.06	0.55
1:E:295:MET:HE3	1:E:348:TYR:CD1	2.42	0.55
1:A:481:SER:O	1:A:497:ARG:HD2	2.07	0.55
1:B:244:ARG:HD2	1:B:280:GLU:O	2.06	0.55
1:C:362:ARG:HD2	1:C:401:ASP:OD2	2.06	0.55
1:D:149:ASP:OD2	1:F:169:TYR:OH	2.25	0.55
1:B:156:ARG:NH2	1:B:334:GLU:OE1	2.40	0.55
1:F:134:ASP:N	1:F:135:PRO:CD	2.70	0.55
1:F:146:SER:O	1:F:175:GLN:HB2	2.07	0.55
1:E:103:ASP:HB3	1:E:107:ARG:HH21	1.72	0.54
1:E:145:TRP:CZ2	1:E:173:ARG:HD3	2.42	0.54
1:F:76:ARG:HD3	1:F:184:HIS:CG	2.42	0.54
1:H:104:GLU:OE1	1:H:108:ARG:NH1	2.39	0.54
1:A:48:ARG:NH2	1:A:100:GLU:OE1	2.38	0.54
1:D:421:ARG:NH2	1:G:420:ASP:OD2	2.35	0.54
1:H:311:GLN:HE21	1:H:311:GLN:HA	1.72	0.54
1:B:144:MET:HE3	1:B:189:ASN:HA	1.89	0.54
1:C:498:GLU:HB3	1:C:503:ARG:HG2	1.90	0.54
1:E:405:LEU:O	1:E:405:LEU:HD22	2.08	0.54
1:F:470:ILE:HD13	1:F:532:CYS:HB3	1.89	0.54
1:G:144:MET:HE3	1:G:189:ASN:HA	1.88	0.54
1:C:69:PRO:HD3	1:C:115:ASP:HB2	1.89	0.54
1:D:218:ALA:N	1:D:259:GLU:OE1	2.30	0.54
1:F:76:ARG:HG2	1:F:184:HIS:CE1	2.41	0.54
1:H:324:PHE:CD1	1:H:326:ARG:HG2	2.43	0.54
1:B:85:TYR:CE2	1:B:199:MET:HE1	2.43	0.54
1:C:17:PRO:C	1:C:18:ARG:HG3	2.32	0.54
1:D:358:ILE:H	1:D:359:GLY:HA3	1.72	0.54
1:F:286:HIS:O	1:F:289:VAL:HG12	2.07	0.54
1:H:163:GLU:OE2	1:H:183:SER:N	2.40	0.54
1:B:500:GLY:O	1:B:501:ASP:HB2	2.08	0.53
1:C:338:ASP:OD2	1:C:341:ARG:NH2	2.31	0.53
1:F:190:TYR:OH	1:F:199:MET:HG3	2.07	0.53
1:F:481:SER:O	1:F:497:ARG:HD2	2.08	0.53
1:H:498:GLU:CD	1:H:523:ARG:HH21	2.16	0.53
1:C:363:ARG:NH1	1:C:393:TYR:O	2.42	0.53
1:D:69:PRO:HD3	1:D:115:ASP:HB2	1.91	0.53
1:H:200:LEU:HB3	1:H:201:GLU:C	2.34	0.53
1:D:363:ARG:NH1	1:D:393:TYR:O	2.42	0.53
1:F:239:TYR:O	1:F:243:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:OD1	1:B:40:ASN:N	2.41	0.53
1:D:324:PHE:CD1	1:D:326:ARG:HG2	2.44	0.53
1:E:144:MET:HB2	1:E:178:TRP:HB3	1.90	0.53
1:E:268:VAL:HG23	1:E:315:ILE:HG22	1.91	0.53
1:G:467:MET:HE2	1:G:533:MET:SD	2.47	0.53
1:C:44:THR:HG21	1:C:91:GLU:CG	2.39	0.53
1:F:28:PHE:HB2	1:F:390:VAL:HG22	1.91	0.53
1:B:104:GLU:OE1	1:B:108:ARG:NH1	2.41	0.53
1:C:263:TRP:CD2	1:C:264:PRO:HD2	2.44	0.53
1:H:215:ARG:HD2	1:H:285:PHE:CE2	2.44	0.53
1:A:328:HIS:NE2	1:A:358:ILE:O	2.41	0.52
1:H:162:THR:HG22	1:H:163:GLU:HG3	1.91	0.52
1:H:192:ASN:OD1	1:H:194:ALA:N	2.36	0.52
1:B:40:ASN:ND2	1:B:42:ASP:CG	2.67	0.52
1:F:127:TRP:O	1:F:128:PHE:C	2.53	0.52
1:E:246:GLU:OE2	1:E:249:ARG:NH1	2.42	0.52
1:D:44:THR:HG21	1:D:91:GLU:OE1	2.09	0.52
1:D:81:ASP:OD1	1:D:81:ASP:N	2.40	0.52
1:F:525:GLU:OE2	1:F:543:GLU:HG2	2.08	0.52
1:G:74:PRO:HD3	1:G:83:SER:OG	2.10	0.52
1:B:38:ASP:OD1	1:B:40:ASN:OD1	2.26	0.52
1:G:295:MET:HE1	1:G:351:ASP:HB2	1.91	0.52
1:F:156:ARG:HH21	1:F:158:ILE:HA	1.74	0.52
1:A:263:TRP:CD2	1:A:264:PRO:HD2	2.44	0.52
1:A:362:ARG:HB2	1:A:367:LEU:HD13	1.92	0.52
1:D:358:ILE:H	1:D:359:GLY:CA	2.23	0.52
1:G:343:TYR:CE2	1:G:344:MET:HE3	2.45	0.52
1:A:66:TRP:C	1:A:66:TRP:CD1	2.87	0.52
1:B:289:VAL:HG11	1:B:323:ILE:HG22	1.91	0.52
1:G:474:HIS:CE1	1:G:559:VAL:HG21	2.45	0.52
1:B:408:ARG:O	1:B:409:ASP:HB3	2.10	0.51
1:E:120:HIS:CD2	1:E:185:GLN:HB3	2.46	0.51
1:E:407:ASP:C	1:E:409:ASP:N	2.68	0.51
1:H:34:ARG:HG3	1:H:44:THR:HG23	1.93	0.51
1:D:34:ARG:HG3	1:D:44:THR:HG23	1.92	0.51
1:D:429:ASP:OD1	1:G:455:ARG:NH2	2.43	0.51
1:B:69:PRO:HD3	1:B:115:ASP:HB2	1.92	0.51
1:B:362:ARG:NH2	1:B:403:ILE:HD11	2.25	0.51
1:C:440:ASP:OD2	1:C:442:ILE:N	2.32	0.51
1:C:44:THR:HG21	1:C:91:GLU:HG2	1.92	0.51
1:C:200:LEU:O	1:C:204:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:TYR:CD2	1:C:435:LEU:HD13	2.45	0.51
1:D:355:LYS:HE3	1:D:367:LEU:CD2	2.41	0.51
1:E:470:ILE:HD13	1:E:473:ARG:NH2	2.25	0.51
1:F:117:VAL:HG11	1:F:120:HIS:HE1	1.72	0.51
1:F:276:THR:HG21	1:F:279:ASP:HB3	1.93	0.51
1:G:190:TYR:O	1:G:196:GLN:NE2	2.44	0.51
1:H:95:LEU:N	1:H:95:LEU:HD12	2.25	0.51
1:H:353:ARG:NH2	1:H:368:LEU:HA	2.25	0.51
1:E:117:VAL:HA	1:E:217:ASP:HB2	1.92	0.51
1:H:200:LEU:HG	1:H:202:VAL:HA	1.91	0.51
1:H:304:PRO:HG3	1:H:344:MET:HE3	1.92	0.51
1:E:498:GLU:OE2	1:E:523:ARG:NH1	2.44	0.51
1:F:137:GLY:N	1:F:139:TYR:N	2.54	0.51
1:A:81:ASP:OD1	1:A:81:ASP:N	2.44	0.51
1:H:66:TRP:CZ3	1:H:390:VAL:HG11	2.45	0.51
1:H:351:ASP:HB3	1:H:354:MET:O	2.10	0.51
1:E:304:PRO:HG3	1:E:344:MET:HE3	1.92	0.51
1:D:102:VAL:O	1:D:106:HIS:ND1	2.43	0.50
1:H:80:TYR:CD1	1:H:331:LEU:HD21	2.46	0.50
1:D:117:VAL:HA	1:D:217:ASP:HB2	1.92	0.50
1:E:184:HIS:CD2	1:E:185:GLN:HG3	2.42	0.50
1:F:170:ASP:HB2	1:F:173:ARG:HE	1.76	0.50
1:C:324:PHE:CD1	1:C:326:ARG:HG2	2.46	0.50
1:D:263:TRP:CD2	1:D:264:PRO:HD2	2.46	0.50
1:D:359:GLY:O	1:D:407:ASP:HB3	2.11	0.50
1:H:203:LEU:HB3	1:H:207:LEU:HD12	1.93	0.50
1:C:257:LEU:HG	1:C:283:MET:HB2	1.92	0.50
1:F:69:PRO:HD3	1:F:115:ASP:HB2	1.93	0.50
1:F:128:PHE:O	1:F:129:GLN:C	2.54	0.50
1:H:351:ASP:HB3	1:H:352:PRO:CA	2.41	0.50
1:G:196:GLN:O	1:G:200:LEU:HD13	2.11	0.50
1:C:339:GLU:HG2	1:C:345:TYR:CZ	2.46	0.50
1:F:362:ARG:HH11	1:F:401:ASP:CG	2.20	0.50
1:G:259:GLU:HG3	1:G:331:LEU:HD13	1.93	0.50
1:E:481:SER:O	1:E:497:ARG:HD2	2.11	0.50
1:F:440:ASP:OD1	1:F:442:ILE:N	2.26	0.50
1:E:132:ARG:CB	1:E:173:ARG:HG3	2.42	0.49
1:F:136:ASP:HB2	1:F:137:GLY:C	2.37	0.49
1:F:137:GLY:H	1:F:139:TYR:N	2.03	0.49
1:H:121:THR:HG22	1:H:122:SER:O	2.11	0.49
1:F:128:PHE:C	1:F:130:ALA:N	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ASP:C	1:F:134:ASP:OD1	2.56	0.49
1:F:413:THR:HG21	1:F:438:ILE:HG13	1.94	0.49
1:G:473:ARG:C	1:G:474:HIS:CD2	2.91	0.49
1:H:215:ARG:HD2	1:H:285:PHE:HE2	1.77	0.49
1:E:257:LEU:HG	1:E:283:MET:HB2	1.94	0.49
1:E:404:TRP:CD1	1:H:436:PRO:HD3	2.48	0.49
1:F:129:GLN:O	1:F:132:ARG:HG3	2.12	0.49
1:B:362:ARG:HD2	1:B:401:ASP:OD2	2.13	0.49
1:C:343:TYR:CZ	1:C:344:MET:HE3	2.47	0.49
1:E:135:PRO:HB3	1:E:173:ARG:NH1	2.27	0.49
1:F:324:PHE:CD1	1:F:326:ARG:HG2	2.47	0.49
1:F:402:ASN:C	1:F:410:SER:HB2	2.37	0.49
1:H:201:GLU:HB3	1:H:204:ARG:HG2	1.93	0.49
1:E:239:TYR:O	1:E:242:ARG:HB2	2.12	0.49
1:H:199:MET:O	1:H:201:GLU:N	2.43	0.49
1:F:405:LEU:HB2	1:F:410:SER:HB3	1.95	0.49
1:A:28:PHE:HB2	1:A:390:VAL:HG22	1.95	0.49
1:F:190:TYR:HA	1:F:195:VAL:HG21	1.94	0.49
1:H:40:ASN:HD22	1:H:46:ASP:CG	2.20	0.49
1:E:343:TYR:CE2	1:E:344:MET:HE2	2.48	0.49
1:G:200:LEU:O	1:G:204:ARG:HG3	2.13	0.49
1:H:235:GLU:OE1	1:H:235:GLU:N	2.37	0.49
1:A:360:ILE:HG23	1:A:407:ASP:HA	1.95	0.48
1:E:273:ASP:O	1:E:276:THR:HG22	2.13	0.48
1:G:28:PHE:HB2	1:G:390:VAL:HG22	1.94	0.48
1:H:88:ILE:HG22	1:H:95:LEU:HD12	1.95	0.48
1:H:132:ARG:HG3	1:H:135:PRO:HG3	1.95	0.48
1:G:125:HIS:HD2	1:G:127:TRP:HB2	1.77	0.48
1:G:409:ASP:C	1:G:411:VAL:N	2.69	0.48
1:E:298:ARG:HH11	1:E:299:ARG:HH21	1.62	0.48
1:H:32:LEU:HD22	1:H:412:ARG:HB3	1.95	0.48
1:H:223:TYR:HD2	1:H:236:THR:HG22	1.78	0.48
1:A:244:ARG:HD2	1:A:280:GLU:O	2.12	0.48
1:A:349:ALA:C	1:A:351:ASP:H	2.20	0.48
1:E:169:TYR:HA	1:E:176:TYR:HA	1.96	0.48
1:G:498:GLU:OE1	1:G:523:ARG:NH1	2.40	0.48
1:H:416:GLN:HG2	1:H:445:TYR:HB3	1.95	0.48
1:A:530:VAL:HG22	1:A:537:GLN:HG2	1.94	0.48
1:F:74:PRO:HD3	1:F:83:SER:OG	2.13	0.48
1:G:217:ASP:HB3	1:G:331:LEU:HD21	1.96	0.48
1:H:258:ALA:HB2	1:H:281:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:MET:HG3	1:H:357:ASN:CG	2.38	0.48
1:D:329:ASP:O	1:D:333:LEU:HA	2.14	0.48
1:D:386:PRO:HA	1:D:497:ARG:NH2	2.29	0.48
1:G:287:PHE:CE1	1:G:324:PHE:HZ	2.32	0.48
1:G:500:GLY:O	1:G:501:ASP:HB2	2.13	0.48
1:E:190:TYR:OH	1:E:199:MET:HG2	2.14	0.48
1:H:292:ARG:HG3	1:H:308:ILE:HG12	1.96	0.48
1:H:354:MET:C	1:H:357:ASN:OD1	2.56	0.48
1:D:243:VAL:O	1:D:247:VAL:HG13	2.14	0.47
1:E:81:ASP:OD1	1:E:81:ASP:N	2.44	0.47
1:F:129:GLN:HE22	1:F:173:ARG:NH1	2.12	0.47
1:A:298:ARG:NH1	1:A:351:ASP:OD2	2.47	0.47
1:B:420:ASP:OD1	1:F:421:ARG:HB2	2.14	0.47
1:B:217:ASP:HB3	1:B:331:LEU:HD21	1.95	0.47
1:F:83:SER:O	1:F:126:PRO:HD2	2.13	0.47
1:F:179:HIS:HA	1:F:187:ASP:OD1	2.13	0.47
1:G:189:ASN:O	1:G:195:VAL:HG21	2.14	0.47
1:G:498:GLU:CD	1:G:523:ARG:HH22	2.22	0.47
1:H:481:SER:O	1:H:497:ARG:HD2	2.14	0.47
1:C:362:ARG:CB	1:C:367:LEU:HD13	2.43	0.47
1:G:85:TYR:CE2	1:G:199:MET:HE1	2.50	0.47
1:H:197:GLU:HG3	1:H:198:ALA:H	1.80	0.47
1:H:326:ARG:HB2	1:H:361:ARG:HH12	1.78	0.47
1:A:344:MET:HE2	1:A:347:GLU:HG3	1.97	0.47
1:D:104:GLU:HG3	1:D:108:ARG:NH1	2.30	0.47
1:D:121:THR:O	1:D:186:PRO:HD2	2.15	0.47
1:D:263:TRP:CG	1:D:264:PRO:HD2	2.49	0.47
1:E:134:ASP:HA	1:E:135:PRO:HD2	1.81	0.47
1:E:305:ILE:O	1:E:309:MET:HG2	2.15	0.47
1:G:474:HIS:CE1	1:G:559:VAL:CG2	2.98	0.47
1:H:167:TRP:CZ3	1:H:177:TYR:O	2.67	0.47
1:A:40:ASN:ND2	1:A:42:ASP:CG	2.73	0.47
1:B:351:ASP:HB3	1:B:354:MET:HB3	1.97	0.47
1:C:155:ALA:HB1	1:C:180:ARG:NH1	2.29	0.47
1:D:244:ARG:HD2	1:D:280:GLU:O	2.15	0.47
1:H:28:PHE:HB2	1:H:390:VAL:HG22	1.97	0.47
1:C:299:ARG:NH2	1:C:301:GLN:OE1	2.48	0.47
1:E:66:TRP:CD1	1:E:66:TRP:C	2.93	0.47
1:F:189:ASN:O	1:F:195:VAL:HG21	2.15	0.47
1:A:362:ARG:HD2	1:A:401:ASP:OD2	2.14	0.47
1:F:40:ASN:OD1	1:F:46:ASP:OD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:365:ALA:HB3	1:H:366:PRO:HD3	1.97	0.47
1:A:404:TRP:CD1	1:C:436:PRO:HD3	2.50	0.46
1:C:127:TRP:HZ3	1:C:199:MET:HE2	1.80	0.46
1:H:199:MET:O	1:H:202:VAL:HG23	2.15	0.46
1:C:197:GLU:O	1:C:201:GLU:HB2	2.14	0.46
1:E:127:TRP:HZ3	1:E:199:MET:HE1	1.79	0.46
1:E:402:ASN:C	1:E:403:ILE:O	2.57	0.46
1:F:145:TRP:CZ3	1:F:177:TYR:HB3	2.50	0.46
1:H:163:GLU:OE1	1:H:182:PHE:HA	2.15	0.46
1:H:225:ARG:HH21	1:H:234:PRO:HD2	1.80	0.46
1:F:188:LEU:CD1	1:F:199:MET:HE3	2.46	0.46
1:B:344:MET:HE2	1:B:347:GLU:HG3	1.98	0.46
1:D:144:MET:HE3	1:D:189:ASN:HA	1.97	0.46
1:E:298:ARG:CZ	1:E:351:ASP:HB2	2.46	0.46
1:G:239:TYR:O	1:G:243:VAL:HG23	2.15	0.46
1:H:72:GLN:HA	1:H:89:LEU:HD13	1.96	0.46
1:H:190:TYR:OH	1:H:199:MET:HG2	2.15	0.46
1:H:244:ARG:HD3	1:H:280:GLU:O	2.15	0.46
1:A:513:PHE:HE1	1:H:466:LYS:NZ	2.14	0.46
1:D:144:MET:HB2	1:D:178:TRP:HB3	1.97	0.46
1:A:117:VAL:HA	1:A:217:ASP:HB2	1.97	0.46
1:C:239:TYR:O	1:C:243:VAL:HG23	2.15	0.46
1:D:358:ILE:N	1:D:359:GLY:CA	2.79	0.46
1:D:421:ARG:HB2	1:G:420:ASP:OD1	2.15	0.46
1:H:66:TRP:CD1	1:H:66:TRP:C	2.94	0.46
1:H:81:ASP:OD1	1:H:81:ASP:N	2.48	0.46
1:C:117:VAL:HA	1:C:217:ASP:HB2	1.98	0.46
1:F:159:PHE:C	1:F:161:ASP:H	2.24	0.46
1:C:47:LEU:O	1:C:51:ILE:HG13	2.16	0.46
1:G:131:SER:O	1:G:173:ARG:NH1	2.47	0.46
1:H:119:ASN:ND2	1:H:221:TYR:HB2	2.31	0.46
1:B:324:PHE:CD1	1:B:326:ARG:HG2	2.50	0.46
1:C:324:PHE:HB3	1:C:390:VAL:HB	1.98	0.46
1:G:500:GLY:C	1:G:502:ASP:H	2.24	0.46
1:A:295:MET:HE1	1:A:351:ASP:CG	2.40	0.45
1:D:116:LEU:HD22	1:D:118:MET:HE3	1.98	0.45
1:F:146:SER:O	1:F:176:TYR:N	2.49	0.45
1:A:397:ILE:HG22	1:A:461:LEU:HB2	1.97	0.45
1:F:167:TRP:CE2	1:F:178:TRP:HE3	2.34	0.45
1:F:237:HIS:CE1	1:F:269:GLU:HB3	2.51	0.45
1:A:367:LEU:HD12	1:A:367:LEU:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LYS:HG2	1:B:320:GLN:HG2	1.97	0.45
1:C:402:ASN:HB3	1:C:405:LEU:HD22	1.98	0.45
1:E:413:THR:HG23	1:E:414:PRO:HD2	1.97	0.45
1:F:126:PRO:C	1:F:127:TRP:O	2.55	0.45
1:H:357:ASN:O	1:H:357:ASN:ND2	2.50	0.45
1:E:413:THR:HG21	1:E:438:ILE:HG13	1.98	0.45
1:G:69:PRO:HD3	1:G:115:ASP:HB2	1.98	0.45
1:G:146:SER:C	1:G:148:THR:H	2.25	0.45
1:G:154:ASP:HB2	1:G:228:THR:O	2.16	0.45
1:D:396:GLU:HG2	1:D:397:ILE:HG23	1.99	0.45
1:G:498:GLU:OE2	1:G:503:ARG:NH1	2.50	0.45
1:B:246:GLU:OE2	1:B:249:ARG:NH1	2.50	0.45
1:C:300:GLU:OE2	1:C:512:ARG:NH1	2.48	0.45
1:C:453:GLN:HB3	1:C:461:LEU:HB3	1.99	0.45
1:G:237:HIS:NE2	1:G:269:GLU:HG2	2.32	0.45
1:G:308:ILE:O	1:G:312:THR:OG1	2.23	0.45
1:H:358:ILE:HD13	1:H:358:ILE:HA	1.88	0.45
1:A:467:MET:HE1	1:A:555:PHE:CE2	2.51	0.45
1:D:128:PHE:CE2	1:D:132:ARG:HD3	2.52	0.45
1:F:171:PRO:HD2	1:F:173:ARG:NH2	2.31	0.45
1:F:268:VAL:HG23	1:F:315:ILE:HG22	1.98	0.45
1:F:279:ASP:OD1	1:F:279:ASP:N	2.50	0.45
1:C:235:GLU:OE1	1:C:235:GLU:N	2.44	0.45
1:C:408:ARG:HG2	1:C:408:ARG:HH11	1.81	0.45
1:E:466:LYS:NZ	1:E:533:MET:O	2.24	0.45
1:H:117:VAL:HA	1:H:217:ASP:HB2	1.98	0.45
1:H:200:LEU:HD12	1:H:204:ARG:HG3	1.99	0.45
1:C:83:SER:O	1:C:126:PRO:HD2	2.17	0.45
1:F:128:PHE:C	1:F:130:ALA:H	2.25	0.45
1:H:290:MET:HB3	1:H:291:PRO:HD3	1.99	0.45
1:H:470:ILE:HG21	1:H:532:CYS:HB3	1.99	0.45
1:B:215:ARG:HD3	1:B:217:ASP:OD1	2.18	0.44
1:D:289:VAL:O	1:D:293:ILE:HG13	2.17	0.44
1:H:55:ASP:OD1	1:H:55:ASP:N	2.49	0.44
1:C:306:SER:OG	1:C:484:GLU:OE2	2.32	0.44
1:E:295:MET:HE3	1:E:348:TYR:HD1	1.82	0.44
1:G:223:TYR:H	1:G:236:THR:HG22	1.82	0.44
1:H:522:ARG:CZ	1:H:543:GLU:HG2	2.47	0.44
1:B:48:ARG:NH1	1:B:100:GLU:OE2	2.46	0.44
1:E:157:ILE:O	1:E:160:VAL:HG22	2.17	0.44
1:A:69:PRO:HD3	1:A:115:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:HIS:CE1	1:B:269:GLU:HB3	2.53	0.44
1:C:188:LEU:CD1	1:C:199:MET:HE3	2.48	0.44
1:D:298:ARG:NH2	1:D:350:LYS:O	2.50	0.44
1:E:407:ASP:OD1	1:E:408:ARG:N	2.49	0.44
1:G:192:ASN:O	1:G:195:VAL:HG22	2.18	0.44
1:D:355:LYS:HB2	1:D:355:LYS:HE2	1.48	0.44
1:E:145:TRP:CZ3	1:E:177:TYR:HB3	2.52	0.44
1:H:295:MET:HE3	1:H:348:TYR:CD1	2.53	0.44
1:A:151:LYS:HB2	1:A:151:LYS:HE3	1.63	0.44
1:A:217:ASP:HB3	1:A:331:LEU:HD21	1.99	0.44
1:B:265:ALA:H	1:B:267:VAL:H	1.65	0.44
1:B:409:ASP:HA	1:B:412:ARG:HD2	2.00	0.44
1:H:95:LEU:HD12	1:H:95:LEU:H	1.82	0.44
1:C:66:TRP:CD1	1:C:66:TRP:C	2.96	0.44
1:D:297:VAL:HG13	1:D:553:HIS:HE1	1.83	0.44
1:D:466:LYS:HD3	1:D:533:MET:CE	2.48	0.44
1:F:38:ASP:OD1	1:F:40:ASN:OD1	2.35	0.44
1:F:171:PRO:O	1:F:173:ARG:N	2.43	0.44
1:H:203:LEU:HG	1:H:214:PHE:CE1	2.53	0.44
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.84	0.44
1:C:408:ARG:HG2	1:C:408:ARG:NH1	2.32	0.44
1:E:509:ASN:O	1:E:553:HIS:HA	2.18	0.44
1:H:125:HIS:HD2	1:H:127:TRP:HB2	1.82	0.44
1:B:149:ASP:OD1	1:B:149:ASP:C	2.60	0.44
1:C:40:ASN:OD1	1:C:40:ASN:N	2.50	0.44
1:D:351:ASP:C	1:D:353:ARG:N	2.71	0.44
1:E:30:GLU:OE1	1:E:326:ARG:NH2	2.38	0.44
1:E:359:GLY:HA3	1:E:408:ARG:NH1	2.33	0.44
1:E:403:ILE:C	1:E:405:LEU:H	2.20	0.44
1:F:125:HIS:ND1	1:F:126:PRO:HD2	2.30	0.44
1:G:386:PRO:HG3	1:G:482:TYR:HB2	1.99	0.44
1:H:295:MET:HG2	1:H:344:MET:SD	2.58	0.44
1:B:474:HIS:HB3	1:B:476:VAL:HG12	1.99	0.43
1:C:409:ASP:C	1:C:411:VAL:N	2.75	0.43
1:E:407:ASP:CG	1:E:410:SER:H	2.13	0.43
1:A:200:LEU:O	1:A:204:ARG:HG3	2.18	0.43
1:F:150:ASP:CG	1:F:151:LYS:H	2.22	0.43
1:G:66:TRP:CD1	1:G:66:TRP:C	2.95	0.43
1:F:85:TYR:CE2	1:F:199:MET:HE1	2.53	0.43
1:H:66:TRP:HZ3	1:H:390:VAL:HG11	1.82	0.43
1:C:405:LEU:O	1:C:406:GLY:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PHE:HB3	1:E:390:VAL:HB	1.99	0.43
1:F:133:THR:CG2	1:F:134:ASP:HA	2.36	0.43
1:H:123:ASP:OD1	1:H:124:GLN:NE2	2.44	0.43
1:B:40:ASN:OD1	1:B:46:ASP:OD2	2.36	0.43
1:E:24:LYS:HA	1:E:320:GLN:HE21	1.82	0.43
1:E:244:ARG:HD3	1:E:280:GLU:O	2.19	0.43
1:F:190:TYR:HA	1:F:195:VAL:CG2	2.49	0.43
1:F:528:THR:HG21	1:F:537:GLN:OE1	2.18	0.43
1:G:228:THR:HB	1:G:229:ASN:H	1.51	0.43
1:H:71:TYR:OH	1:H:115:ASP:O	2.30	0.43
1:H:363:ARG:HG3	1:H:411:VAL:CG2	2.49	0.43
1:C:290:MET:HB3	1:C:291:PRO:HD3	2.01	0.43
1:D:132:ARG:NH1	1:D:170:ASP:OD1	2.52	0.43
1:D:327:ASN:O	1:D:335:MET:HG3	2.18	0.43
1:G:104:GLU:HA	1:G:107:ARG:HD2	2.01	0.43
1:H:192:ASN:O	1:H:195:VAL:HG22	2.18	0.43
1:A:38:ASP:OD1	1:A:40:ASN:OD1	2.36	0.43
1:C:496:VAL:HG12	1:C:498:GLU:HG2	2.01	0.43
1:E:179:HIS:HA	1:E:187:ASP:OD1	2.19	0.43
1:F:235:GLU:OE1	1:F:235:GLU:N	2.48	0.43
1:H:303:TYR:HB2	1:H:304:PRO:HD3	2.01	0.43
1:H:429:ASP:OD1	1:H:430:PRO:HD2	2.19	0.43
1:G:324:PHE:CD1	1:G:326:ARG:HG2	2.54	0.43
1:H:91:GLU:H	1:H:91:GLU:HG2	1.39	0.43
1:H:416:GLN:HE21	1:H:445:TYR:CA	2.31	0.43
1:D:290:MET:HB3	1:D:291:PRO:HD3	2.00	0.43
1:H:88:ILE:HG21	1:H:94:ASP:HA	2.01	0.43
1:A:333:LEU:HD21	1:A:408:ARG:HB2	2.00	0.43
1:A:509:ASN:O	1:A:553:HIS:HA	2.17	0.43
1:B:85:TYR:HD1	1:B:116:LEU:HD11	1.84	0.43
1:B:409:ASP:O	1:B:410:SER:HB3	2.19	0.43
1:C:408:ARG:O	1:C:409:ASP:CB	2.63	0.43
1:D:287:PHE:CE1	1:D:324:PHE:HZ	2.36	0.43
1:E:89:LEU:HA	1:E:90:PRO:HD3	1.83	0.43
1:F:54:LEU:HD23	1:F:54:LEU:HA	1.84	0.43
1:G:365:ALA:HB3	1:G:366:PRO:HD3	2.01	0.43
1:H:531:GLU:CD	1:H:533:MET:H	2.26	0.43
1:B:103:ASP:HB3	1:B:107:ARG:HH12	1.83	0.42
1:B:203:LEU:HD22	1:B:214:PHE:CE1	2.54	0.42
1:C:437:VAL:O	1:C:439:MET:HG3	2.19	0.42
1:E:47:LEU:O	1:E:51:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:ASP:OD1	1:F:81:ASP:N	2.52	0.42
1:B:414:PRO:HG3	1:B:434:TYR:CE1	2.55	0.42
1:B:498:GLU:CD	1:B:523:ARG:HH12	2.27	0.42
1:C:305:ILE:O	1:C:308:ILE:HG13	2.19	0.42
1:D:276:THR:HG21	1:D:279:ASP:HB3	2.00	0.42
1:E:365:ALA:HB3	1:E:366:PRO:HD3	2.01	0.42
1:H:204:ARG:O	1:H:208:ASP:N	2.43	0.42
1:B:286:HIS:CE1	1:B:288:PRO:HG2	2.54	0.42
1:E:143:TYR:HD1	1:E:187:ASP:O	2.02	0.42
1:F:134:ASP:N	1:F:135:PRO:HD3	2.33	0.42
1:H:205:PHE:O	1:H:209:LEU:HG	2.18	0.42
1:A:308:ILE:H	1:A:308:ILE:HG13	1.64	0.42
1:C:54:LEU:HD23	1:C:54:LEU:HA	1.91	0.42
1:D:228:THR:HG21	1:D:233:LEU:HD21	2.01	0.42
1:F:409:ASP:O	1:F:410:SER:CB	2.67	0.42
1:A:339:GLU:HG3	1:A:345:TYR:CD2	2.54	0.42
1:B:481:SER:O	1:B:497:ARG:HD2	2.19	0.42
1:C:367:LEU:HD12	1:C:367:LEU:HA	1.91	0.42
1:E:220:PRO:O	1:E:231:GLU:HA	2.19	0.42
1:E:295:MET:HE2	1:E:295:MET:N	2.34	0.42
1:A:473:ARG:HE	1:A:473:ARG:HB2	1.67	0.42
1:C:200:LEU:HD21	1:C:243:VAL:HG22	2.02	0.42
1:F:151:LYS:HG3	1:F:167:TRP:HZ2	1.85	0.42
1:F:287:PHE:CE1	1:F:324:PHE:HZ	2.37	0.42
1:H:132:ARG:O	1:H:132:ARG:HG2	2.20	0.42
1:H:324:PHE:CE1	1:H:326:ARG:HG2	2.55	0.42
1:E:295:MET:HE3	1:E:348:TYR:CE1	2.54	0.42
1:E:406:GLY:N	1:E:407:ASP:HA	2.35	0.42
1:G:119:ASN:HD22	1:G:120:HIS:HD2	1.66	0.42
1:H:489:ASN:HA	1:H:490:PRO:HD3	1.77	0.42
1:A:372:ARG:HH21	1:A:459:SER:C	2.27	0.42
1:B:329:ASP:OD1	1:B:331:LEU:N	2.49	0.42
1:B:522:ARG:CD	1:B:543:GLU:HG3	2.47	0.42
1:C:340:GLU:HG2	1:C:341:ARG:HG3	2.00	0.42
1:C:407:ASP:C	1:C:408:ARG:HG2	2.45	0.42
1:D:84:ASP:OD2	1:D:87:LYS:HG3	2.20	0.42
1:D:157:ILE:O	1:D:160:VAL:HG22	2.19	0.42
1:E:155:ALA:HB1	1:E:180:ARG:NH1	2.34	0.42
1:D:228:THR:HG23	1:D:230:CYS:H	1.85	0.42
1:D:386:PRO:HG3	1:D:482:TYR:HB2	2.01	0.42
1:F:167:TRP:CH2	1:F:178:TRP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:474:HIS:HE1	1:G:559:VAL:HG21	1.85	0.42
1:C:312:THR:HA	1:C:313:PRO:HD3	1.91	0.42
1:E:76:ARG:HB3	1:E:184:HIS:CE1	2.55	0.42
1:G:148:THR:HG23	1:G:150:ASP:OD1	2.20	0.42
1:H:84:ASP:OD2	1:H:87:LYS:HD3	2.20	0.42
1:H:180:ARG:HD2	1:H:180:ARG:HA	1.87	0.42
1:C:386:PRO:HG3	1:C:482:TYR:HB2	2.01	0.41
1:E:347:GLU:HA	1:E:350:LYS:HE2	2.01	0.41
1:G:204:ARG:HB3	1:G:251:TYR:OH	2.20	0.41
1:A:397:ILE:HB	1:A:453:GLN:HG3	2.02	0.41
1:B:115:ASP:OD1	1:B:215:ARG:HD2	2.20	0.41
1:D:258:ALA:HB2	1:D:281:CYS:SG	2.60	0.41
1:E:265:ALA:O	1:E:268:VAL:HG12	2.21	0.41
1:F:335:MET:HE1	1:F:348:TYR:CD2	2.55	0.41
1:G:481:SER:O	1:G:497:ARG:HD2	2.19	0.41
1:H:88:ILE:HG22	1:H:95:LEU:CD1	2.50	0.41
1:H:200:LEU:O	1:H:201:GLU:CG	2.63	0.41
1:A:135:PRO:HG3	1:A:173:ARG:HD2	2.01	0.41
1:C:178:TRP:CZ2	1:C:180:ARG:HD3	2.55	0.41
1:C:265:ALA:O	1:C:268:VAL:HG12	2.21	0.41
1:G:217:ASP:HA	1:G:259:GLU:HB3	2.02	0.41
1:B:365:ALA:HB3	1:B:366:PRO:HD3	2.02	0.41
1:E:206:TRP:HB2	1:E:214:PHE:HZ	1.84	0.41
1:E:407:ASP:CG	1:E:408:ARG:N	2.78	0.41
1:G:127:TRP:CZ3	1:G:199:MET:HE2	2.52	0.41
1:H:153:PRO:HB2	1:H:154:ASP:H	1.72	0.41
1:D:38:ASP:HB3	1:D:426:SER:HB2	2.02	0.41
1:H:201:GLU:O	1:H:202:VAL:C	2.62	0.41
1:B:44:THR:HG21	1:B:91:GLU:HB2	2.02	0.41
1:C:297:VAL:HG21	1:C:378:PHE:CE1	2.55	0.41
1:D:283:MET:HA	1:D:320:GLN:O	2.21	0.41
1:D:292:ARG:HH12	1:D:307:GLU:HB3	1.86	0.41
1:D:466:LYS:HD3	1:D:533:MET:HE1	2.02	0.41
1:E:263:TRP:CD2	1:E:264:PRO:HD2	2.56	0.41
1:F:40:ASN:ND2	1:F:42:ASP:CG	2.78	0.41
1:F:137:GLY:CA	1:F:139:TYR:H	2.31	0.41
1:G:81:ASP:OD1	1:G:81:ASP:N	2.49	0.41
1:H:488:SER:O	1:H:490:PRO:HD3	2.21	0.41
1:H:194:ALA:CA	1:H:197:GLU:HB3	2.51	0.41
1:A:451:GLU:OE2	1:A:455:ARG:NH1	2.54	0.41
1:E:192:ASN:HA	1:E:193:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:MET:HB3	1:E:291:PRO:HD3	2.02	0.41
1:F:73:SER:H	1:F:89:LEU:HD13	1.86	0.41
1:G:66:TRP:CZ3	1:G:390:VAL:HG11	2.56	0.41
1:G:297:VAL:HG21	1:G:378:PHE:CE1	2.56	0.41
1:H:57:LEU:HD23	1:H:57:LEU:HA	1.84	0.41
1:H:194:ALA:HA	1:H:197:GLU:HB3	2.02	0.41
1:A:323:ILE:HD13	1:A:323:ILE:HG21	1.74	0.41
1:B:48:ARG:NH2	1:B:100:GLU:OE1	2.49	0.41
1:B:66:TRP:CD1	1:B:66:TRP:C	2.98	0.41
1:B:372:ARG:HA	1:B:375:LEU:HD12	2.03	0.41
1:B:440:ASP:HA	1:B:441:PRO:HD3	1.97	0.41
1:C:89:LEU:HA	1:C:90:PRO:HD3	1.83	0.41
1:C:481:SER:O	1:C:497:ARG:HD2	2.20	0.41
1:D:338:ASP:OD1	1:D:338:ASP:C	2.64	0.41
1:E:40:ASN:ND2	1:E:42:ASP:CG	2.79	0.41
1:F:85:TYR:HD1	1:F:116:LEU:HD11	1.86	0.41
1:G:409:ASP:C	1:G:411:VAL:H	2.28	0.41
1:H:181:PHE:HB3	1:H:182:PHE:H	1.76	0.41
1:H:225:ARG:C	1:H:228:THR:HG1	2.26	0.41
1:B:28:PHE:HB2	1:B:390:VAL:HG22	2.03	0.41
1:C:190:TYR:HB3	1:C:223:TYR:CZ	2.56	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.88	0.41
1:E:335:MET:HE1	1:E:348:TYR:CD2	2.56	0.41
1:D:292:ARG:HG3	1:D:308:ILE:HG12	2.03	0.40
1:E:125:HIS:CD2	1:E:127:TRP:H	2.39	0.40
1:F:151:LYS:CG	1:F:167:TRP:CZ2	3.04	0.40
1:H:222:LEU:HB2	1:H:236:THR:HG22	2.03	0.40
1:H:405:LEU:HD13	1:H:435:LEU:HD22	2.03	0.40
1:A:489:ASN:HA	1:A:490:PRO:HD3	1.88	0.40
1:C:40:ASN:OD1	1:C:46:ASP:OD1	2.40	0.40
1:E:371:ASP:CG	1:E:374:GLN:HG3	2.46	0.40
1:G:192:ASN:O	1:G:196:GLN:HG3	2.21	0.40
1:H:144:MET:O	1:H:177:TYR:O	2.39	0.40
1:A:85:TYR:HD1	1:A:116:LEU:HD11	1.86	0.40
1:E:287:PHE:CE1	1:E:329:ASP:HB3	2.56	0.40
1:F:125:HIS:CD2	1:F:127:TRP:HB2	2.55	0.40
1:G:34:ARG:HG3	1:G:44:THR:HG23	2.03	0.40
1:G:188:LEU:CD1	1:G:199:MET:HE3	2.48	0.40
1:G:316:PRO:HB2	1:G:319:CYS:SG	2.61	0.40
1:H:157:ILE:O	1:H:160:VAL:HG12	2.21	0.40
1:H:363:ARG:HG3	1:H:411:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:LEU:HD23	1:C:200:LEU:HA	1.90	0.40
1:C:231:GLU:OE1	1:C:262:GLN:NE2	2.54	0.40
1:C:365:ALA:HB3	1:C:366:PRO:HD3	2.04	0.40
1:A:71:TYR:CZ	1:A:116:LEU:HD13	2.57	0.40
1:A:294:PHE:O	1:A:298:ARG:HG2	2.21	0.40
1:B:81:ASP:OD1	1:B:81:ASP:N	2.51	0.40
1:B:408:ARG:HG2	1:B:409:ASP:H	1.86	0.40
1:C:265:ALA:H	1:C:267:VAL:H	1.68	0.40
1:F:129:GLN:HE22	1:F:173:ARG:HH12	1.68	0.40
1:F:140:GLY:C	1:F:142:PHE:H	2.29	0.40
1:H:40:ASN:OD1	1:H:42:ASP:CG	2.65	0.40
1:H:121:THR:O	1:H:186:PRO:HD2	2.21	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	542/601 (90%)	521 (96%)	17 (3%)	4 (1%)	18	47
1	B	542/601 (90%)	522 (96%)	15 (3%)	5 (1%)	14	41
1	C	542/601 (90%)	513 (95%)	21 (4%)	8 (2%)	8	28
1	D	542/601 (90%)	516 (95%)	21 (4%)	5 (1%)	14	41
1	E	542/601 (90%)	515 (95%)	21 (4%)	6 (1%)	11	36
1	F	542/601 (90%)	496 (92%)	26 (5%)	20 (4%)	2	9
1	G	542/601 (90%)	518 (96%)	16 (3%)	8 (2%)	8	28
1	H	532/601 (88%)	491 (92%)	24 (4%)	17 (3%)	3	11
All	All	4326/4808 (90%)	4092 (95%)	161 (4%)	73 (2%)	7	25

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	ALA
1	A	407	ASP
1	B	150	ASP
1	D	358	ILE
1	E	403	ILE
1	E	411	VAL
1	F	127	TRP
1	F	129	GLN
1	F	131	SER
1	F	149	ASP
1	F	150	ASP
1	F	151	LYS
1	G	226	GLU
1	G	261	ASN
1	G	265	ALA
1	H	153	PRO
1	H	178	TRP
1	H	197	GLU
1	H	198	ALA
1	H	201	GLU
1	H	203	LEU
1	H	230	CYS
1	H	354	MET
1	H	355	LYS
1	H	410	SER
1	A	409	ASP
1	B	265	ALA
1	B	500	GLY
1	C	265	ALA
1	C	333	LEU
1	C	406	GLY
1	D	410	SER
1	E	18	ARG
1	E	265	ALA
1	F	160	VAL
1	F	172	VAL
1	F	265	ALA
1	F	333	LEU
1	G	409	ASP
1	G	410	SER
1	G	500	GLY
1	H	265	ALA
1	H	351	ASP

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Mol	Chain	Res	Type
1	H	500	GLY
1	C	230	CYS
1	C	409	ASP
1	C	410	SER
1	E	500	GLY
1	F	135	PRO
1	F	141	ASP
1	F	187	ASP
1	F	225	ARG
1	G	227	GLY
1	G	408	ARG
1	H	226	GLU
1	B	230	CYS
1	B	409	ASP
1	C	359	GLY
1	D	334	GLU
1	F	173	ARG
1	F	226	GLU
1	H	183	SER
1	H	200	LEU
1	H	359	GLY
1	E	404	TRP
1	F	130	ALA
1	F	138	PRO
1	A	230	CYS
1	F	171	PRO
1	D	500	GLY
1	F	134	ASP
1	C	500	GLY
1	D	264	PRO

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	476/522 (91%)	466 (98%)	10 (2%)	47 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	476/522 (91%)	468 (98%)	8 (2%)	53	83
1	C	476/522 (91%)	464 (98%)	12 (2%)	42	76
1	D	476/522 (91%)	465 (98%)	11 (2%)	44	78
1	E	476/522 (91%)	464 (98%)	12 (2%)	42	76
1	F	476/522 (91%)	455 (96%)	21 (4%)	25	59
1	G	476/522 (91%)	464 (98%)	12 (2%)	42	76
1	H	468/522 (90%)	445 (95%)	23 (5%)	22	55
All	All	3800/4176 (91%)	3691 (97%)	109 (3%)	37	73

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ARG
1	A	308	ILE
1	A	311	GLN
1	A	314	LYS
1	A	324	PHE
1	A	353	ARG
1	A	367	LEU
1	A	401	ASP
1	A	413	THR
1	A	440	ASP
1	B	269	GLU
1	B	410	SER
1	B	413	THR
1	B	448	VAL
1	B	450	VAL
1	B	473	ARG
1	B	483	VAL
1	B	488	SER
1	C	18	ARG
1	C	262	GLN
1	C	308	ILE
1	C	343	TYR
1	C	367	LEU
1	C	401	ASP
1	C	405	LEU
1	C	411	VAL
1	C	432	ARG
1	C	455	ARG

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Mol	Chain	Res	Type
1	C	470	ILE
1	C	498	GLU
1	D	107	ARG
1	D	160	VAL
1	D	164	VAL
1	D	204	ARG
1	D	247	VAL
1	D	262	GLN
1	D	308	ILE
1	D	338	ASP
1	D	355	LYS
1	D	401	ASP
1	D	413	THR
1	E	160	VAL
1	E	173	ARG
1	E	201	GLU
1	E	231	GLU
1	E	298	ARG
1	E	302	ARG
1	E	405	LEU
1	E	411	VAL
1	E	413	THR
1	E	483	VAL
1	E	501	ASP
1	E	544	LEU
1	F	18	ARG
1	F	76	ARG
1	F	102	VAL
1	F	120	HIS
1	F	133	THR
1	F	173	ARG
1	F	228	THR
1	F	231	GLU
1	F	242	ARG
1	F	269	GLU
1	F	308	ILE
1	F	317	GLU
1	F	333	LEU
1	F	343	TYR
1	F	411	VAL
1	F	413	THR
1	F	432	ARG

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Mol	Chain	Res	Type
1	F	439	MET
1	F	455	ARG
1	F	469	GLU
1	F	473	ARG
1	G	39	SER
1	G	148	THR
1	G	164	VAL
1	G	249	ARG
1	G	262	GLN
1	G	308	ILE
1	G	314	LYS
1	G	324	PHE
1	G	333	LEU
1	G	367	LEU
1	G	411	VAL
1	G	413	THR
1	H	18	ARG
1	H	46	ASP
1	H	91	GLU
1	H	104	GLU
1	H	121	THR
1	H	131	SER
1	H	145	TRP
1	H	147	ASP
1	H	151	LYS
1	H	160	VAL
1	H	168	THR
1	H	199	MET
1	H	200	LEU
1	H	215	ARG
1	H	246	GLU
1	H	250	LEU
1	H	308	ILE
1	H	311	GLN
1	H	323	ILE
1	H	358	ILE
1	H	413	THR
1	H	455	ARG
1	H	522	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	125	HIS
1	A	232	ASN
1	A	320	GLN
1	B	52	ASN
1	B	119	ASN
1	B	124	GLN
1	B	416	GLN
1	B	553	HIS
1	C	58	GLN
1	C	328	HIS
1	D	52	ASN
1	D	72	GLN
1	D	119	ASN
1	D	416	GLN
1	D	553	HIS
1	E	58	GLN
1	E	119	ASN
1	E	175	GLN
1	E	184	HIS
1	E	237	HIS
1	E	311	GLN
1	E	320	GLN
1	E	416	GLN
1	E	508	ASN
1	F	58	GLN
1	F	119	ASN
1	F	129	GLN
1	F	166	ASN
1	F	175	GLN
1	F	184	HIS
1	F	318	ASN
1	G	119	ASN
1	G	232	ASN
1	G	261	ASN
1	G	262	GLN
1	G	474	HIS
1	G	508	ASN
1	H	119	ASN
1	H	189	ASN
1	H	311	GLN
1	H	416	GLN
1	H	446	GLN

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Mol	Chain	Res	Type
1	H	553	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/601 (90%)	-0.27	6 (1%) 78 70	13, 24, 43, 71	0
1	B	544/601 (90%)	-0.25	6 (1%) 78 70	12, 25, 48, 72	0
1	C	544/601 (90%)	-0.08	9 (1%) 69 60	14, 31, 51, 102	0
1	D	544/601 (90%)	0.04	14 (2%) 57 47	15, 34, 54, 71	0
1	E	544/601 (90%)	0.14	24 (4%) 39 31	15, 34, 68, 94	0
1	F	544/601 (90%)	0.26	53 (9%) 13 10	14, 31, 87, 103	0
1	G	544/601 (90%)	0.03	14 (2%) 57 47	14, 36, 63, 87	0
1	H	536/601 (89%)	0.45	58 (10%) 11 8	16, 38, 80, 95	0
All	All	4344/4808 (90%)	0.04	184 (4%) 40 32	12, 30, 65, 103	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	169	TYR	10.4
1	D	358	ILE	8.6
1	H	349	ALA	8.1
1	C	406	GLY	7.9
1	H	145	TRP	6.9
1	C	358	ILE	6.9
1	F	164	VAL	6.3
1	D	357	ASN	6.1
1	F	151	LYS	6.0
1	H	358	ILE	5.9
1	F	152	TYR	5.8
1	E	406	GLY	5.6
1	C	407	ASP	5.5
1	H	177	TYR	5.5
1	E	407	ASP	5.5
1	F	144	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	173	ARG	5.0
1	F	228	THR	5.0
1	F	227	GLY	5.0
1	H	357	ASN	4.9
1	H	356	ALA	4.9
1	F	226	GLU	4.9
1	E	405	LEU	4.8
1	D	359	GLY	4.7
1	C	408	ARG	4.7
1	H	198	ALA	4.7
1	F	230	CYS	4.7
1	E	133	THR	4.6
1	H	138	PRO	4.6
1	F	133	THR	4.6
1	H	225	ARG	4.5
1	F	153	PRO	4.5
1	G	333	LEU	4.4
1	H	129	GLN	4.4
1	B	17	PRO	4.3
1	C	17	PRO	4.3
1	F	138	PRO	4.3
1	H	350	LYS	4.2
1	F	174	GLY	4.2
1	H	543	GLU	4.2
1	H	353	ARG	4.2
1	H	352	PRO	4.2
1	F	131	SER	4.2
1	H	154	ASP	4.2
1	F	172	VAL	4.1
1	F	171	PRO	4.1
1	F	165	SER	4.1
1	H	168	THR	4.0
1	F	175	GLN	3.9
1	H	132	ARG	3.9
1	A	350	LYS	3.9
1	F	141	ASP	3.9
1	H	200	LEU	3.8
1	F	166	ASN	3.7
1	H	142	PHE	3.7
1	E	171	PRO	3.7
1	H	199	MET	3.7
1	F	149	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	410	SER	3.7
1	F	135	PRO	3.7
1	H	133	THR	3.6
1	F	225	ARG	3.5
1	F	136	ASP	3.5
1	F	178	TRP	3.5
1	G	358	ILE	3.4
1	B	172	VAL	3.4
1	H	189	ASN	3.4
1	F	142	PHE	3.4
1	H	542	GLY	3.4
1	H	205	PHE	3.4
1	D	352	PRO	3.3
1	G	261	ASN	3.3
1	E	17	PRO	3.3
1	E	169	TYR	3.3
1	H	17	PRO	3.3
1	H	149	ASP	3.3
1	F	148	THR	3.2
1	F	147	ASP	3.2
1	H	153	PRO	3.2
1	F	176	TYR	3.2
1	A	17	PRO	3.2
1	H	135	PRO	3.2
1	F	177	TYR	3.1
1	H	155	ALA	3.1
1	E	173	ARG	3.1
1	A	349	ALA	3.1
1	F	170	ASP	3.0
1	H	202	VAL	3.0
1	E	172	VAL	3.0
1	E	145	TRP	3.0
1	H	188	LEU	3.0
1	G	227	GLY	3.0
1	H	144	MET	2.9
1	H	130	ALA	2.9
1	F	229	ASN	2.9
1	F	221	TYR	2.9
1	F	130	ALA	2.9
1	H	164	VAL	2.9
1	E	136	ASP	2.9
1	H	190	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	354	MET	2.9
1	G	123	ASP	2.8
1	F	146	SER	2.8
1	F	17	PRO	2.8
1	E	175	GLN	2.8
1	H	150	ASP	2.8
1	H	230	CYS	2.7
1	F	167	TRP	2.7
1	D	351	ASP	2.7
1	F	157	ILE	2.7
1	H	165	SER	2.7
1	H	141	ASP	2.7
1	H	167	TRP	2.7
1	F	155	ALA	2.7
1	F	156	ARG	2.6
1	F	134	ASP	2.6
1	H	139	TYR	2.6
1	C	357	ASN	2.6
1	E	164	VAL	2.6
1	D	17	PRO	2.6
1	E	404	TRP	2.6
1	F	128	PHE	2.6
1	G	349	ALA	2.6
1	H	195	VAL	2.6
1	E	408	ARG	2.6
1	F	139	TYR	2.6
1	D	356	ALA	2.6
1	F	129	GLN	2.6
1	H	224	ALA	2.5
1	H	128	PHE	2.5
1	E	276	THR	2.5
1	H	152	TYR	2.5
1	H	151	LYS	2.4
1	G	133	THR	2.4
1	F	353	ARG	2.4
1	A	333	LEU	2.4
1	H	203	LEU	2.4
1	H	140	GLY	2.4
1	H	156	ARG	2.4
1	H	120	HIS	2.4
1	E	147	ASP	2.4
1	F	154	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	135	PRO	2.4
1	A	358	ILE	2.4
1	A	261	ASN	2.4
1	E	103	ASP	2.3
1	D	349	ALA	2.3
1	G	130	ALA	2.3
1	E	132	ARG	2.3
1	H	522	ARG	2.3
1	D	439	MET	2.3
1	D	172	VAL	2.3
1	G	117	VAL	2.3
1	H	233	LEU	2.3
1	E	403	ILE	2.3
1	F	343	TYR	2.3
1	G	226	GLU	2.3
1	H	201	GLU	2.2
1	D	264	PRO	2.2
1	E	129	GLN	2.2
1	B	148	THR	2.2
1	C	439	MET	2.2
1	G	228	THR	2.2
1	H	226	GLU	2.2
1	F	132	ARG	2.2
1	F	140	GLY	2.2
1	B	129	GLN	2.2
1	H	227	GLY	2.2
1	B	409	ASP	2.2
1	C	150	ASP	2.2
1	F	439	MET	2.1
1	E	353	ARG	2.1
1	F	145	TRP	2.1
1	D	150	ASP	2.1
1	G	148	THR	2.1
1	H	185	GLN	2.1
1	G	440	ASP	2.0
1	G	218	ALA	2.0
1	C	264	PRO	2.0
1	D	354	MET	2.0
1	D	333	LEU	2.0
1	H	544	LEU	2.0
1	B	40	ASN	2.0
1	F	189	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.