



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:04 PM UTC

PDB ID : 3PCH / pdb_00003pch
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3-CHLORO-4-HYDROXYBENZOATE
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-01
Resolution : 2.05 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

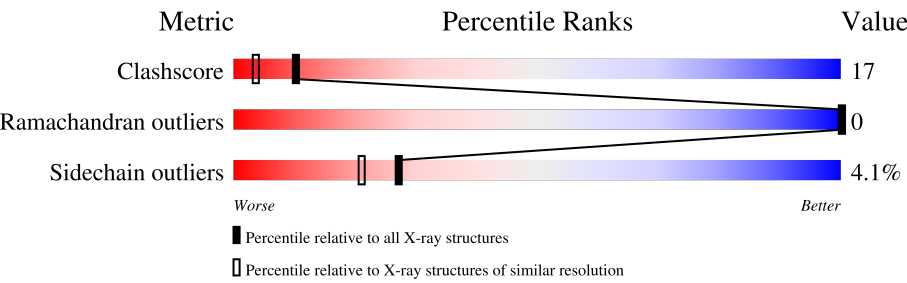
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	60% 32% 6% .
1	B	200	66% 27% 6% .
1	C	200	67% 28% . .
1	D	200	60% 34% 6% .
1	E	200	56% 36% 7% .
1	F	200	61% 32% 6% .
2	M	238	55% 36% 6% ..
2	N	238	68% 24% 6% .

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Mol	Chain	Length	Quality of chain
2	O	238	63%29%5%..
2	P	238	61%30%6%.
2	Q	238	58%34%6%.
2	R	238	58%34%5%..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22080 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 Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

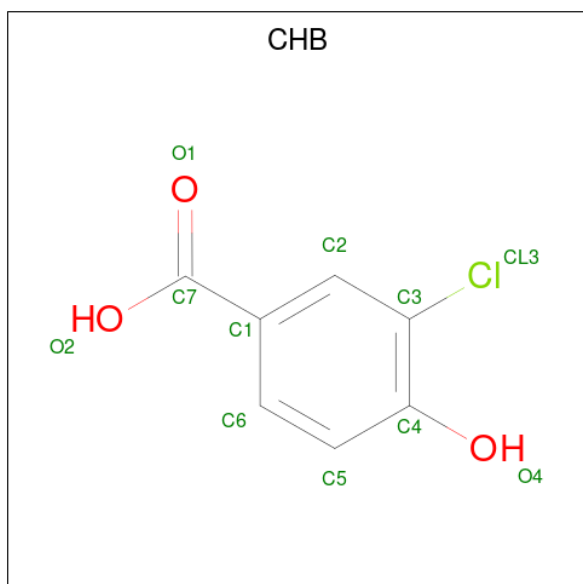
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	N	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	O	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	P	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	Q	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			
2	R	233	Total	C	N	O	S	0	0	0
			1844	1173	334	329	8			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is 3-CHLORO-4-HYDROXYBENZOIC ACID (CCD ID: CHB) (formula: $C_7H_5ClO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C Cl O 11 7 1 3	0	0
4	M	1	Total C Cl O 11 7 1 3	0	0
4	N	1	Total C Cl O 11 7 1 3	0	0
4	N	1	Total C Cl O 11 7 1 3	0	0
4	O	1	Total C Cl O 11 7 1 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	O	1	Total 11	C 7	Cl 1	O 3	0	0
4	P	1	Total 11	C 7	Cl 1	O 3	0	0
4	P	1	Total 11	C 7	Cl 1	O 3	0	0
4	Q	1	Total 11	C 7	Cl 1	O 3	0	0
4	Q	1	Total 11	C 7	Cl 1	O 3	0	0
4	R	1	Total 11	C 7	Cl 1	O 3	0	0
4	R	1	Total 11	C 7	Cl 1	O 3	0	0

- Molecule 5 is water.

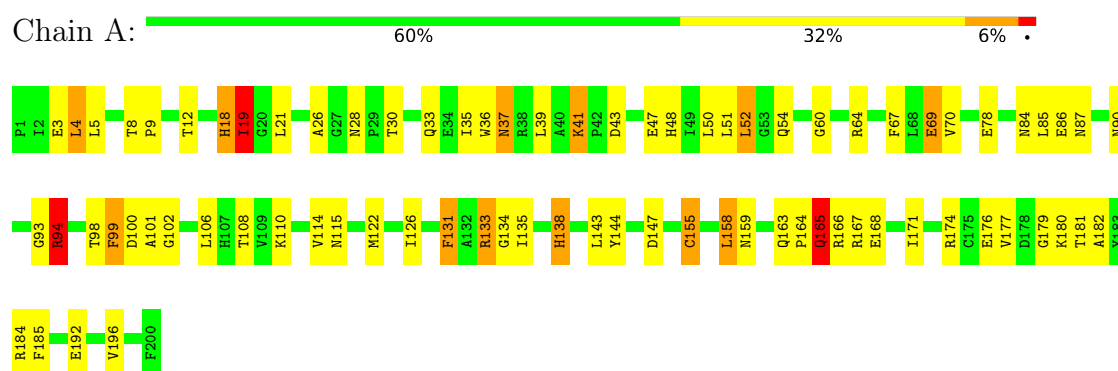
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	M	160	Total 160	O 160	0	0
5	B	83	Total 83	O 83	0	0
5	N	164	Total 164	O 164	0	0
5	C	84	Total 84	O 84	0	0
5	O	155	Total 155	O 155	0	0
5	D	84	Total 84	O 84	0	0
5	P	153	Total 153	O 153	0	0
5	E	83	Total 83	O 83	0	0
5	Q	163	Total 163	O 163	0	0
5	F	83	Total 83	O 83	0	0
5	R	158	Total 158	O 158	0	0

3 Residue-property plots

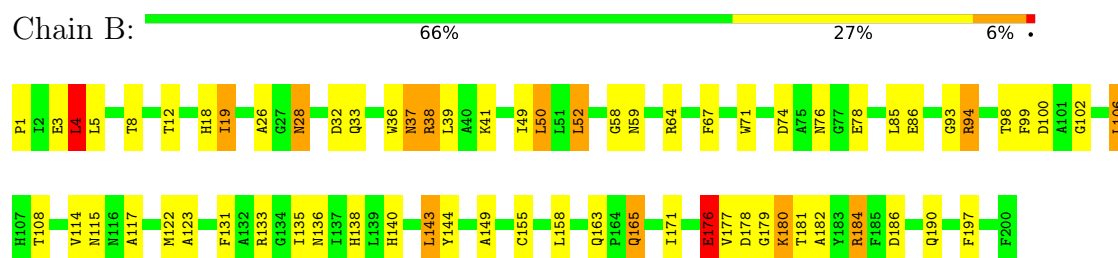
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

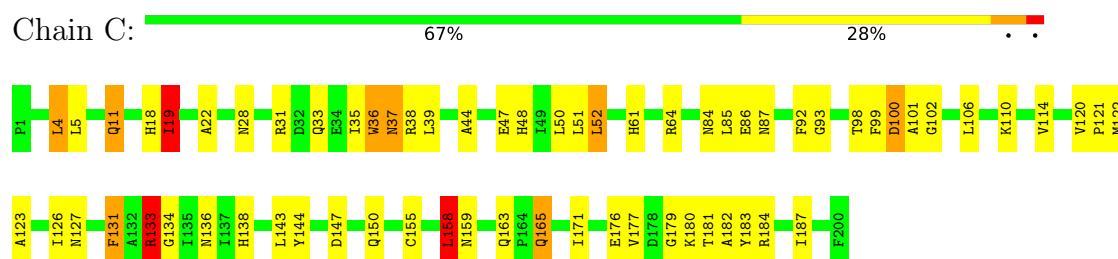
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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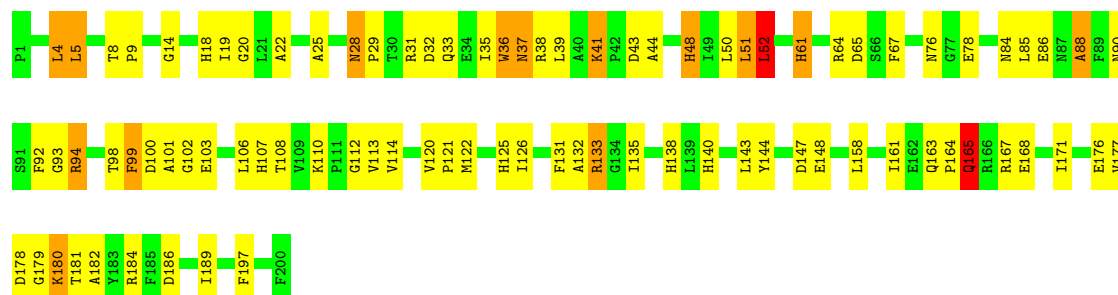
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain





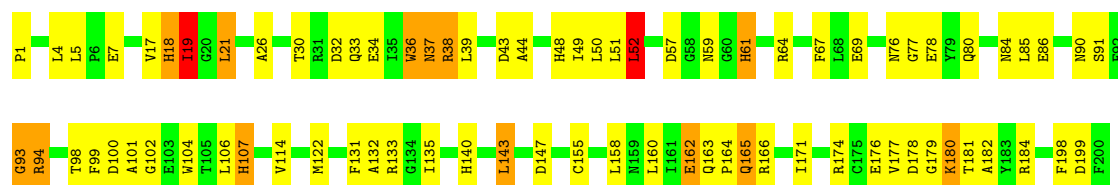
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E: 56% 36% 7% .



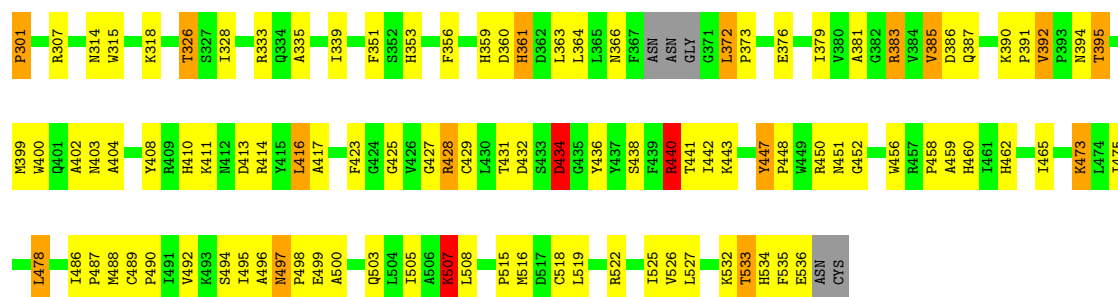
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain F: 61% 32% 6% .



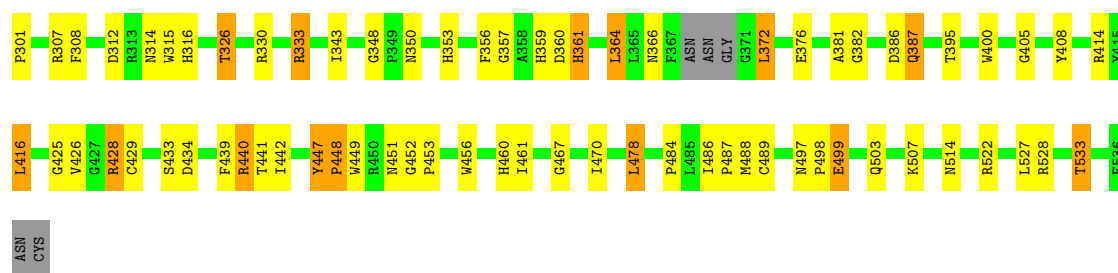
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain M: 55% 36% 6% .



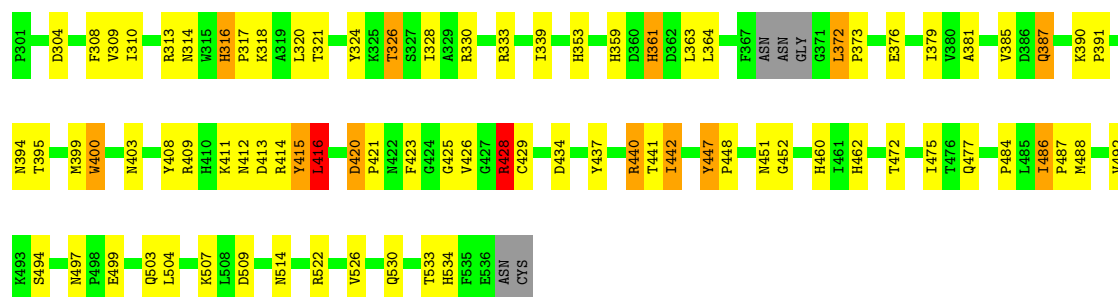
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain N: 68% 24% 6% .



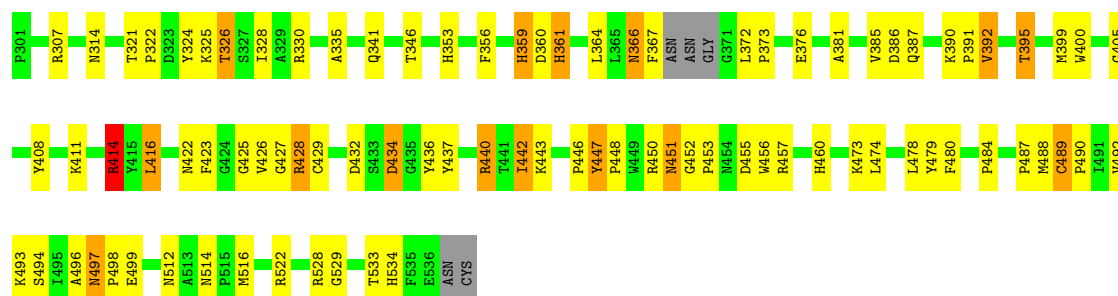
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O: 63% 29% 5% ..



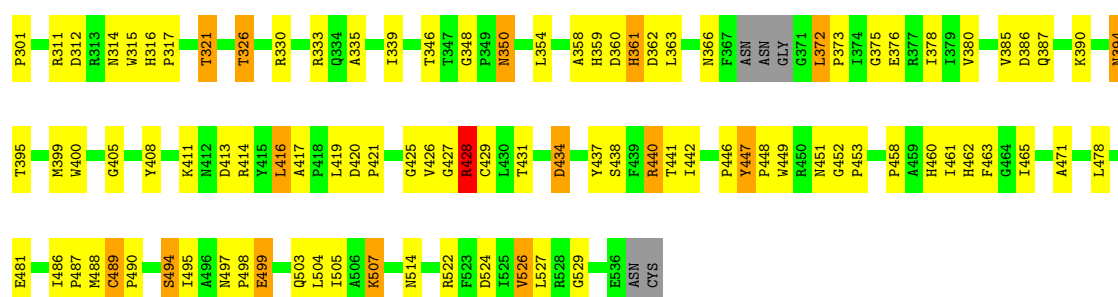
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain P: 61% 30% 6% .



• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain Q: 58% 34% 6% .



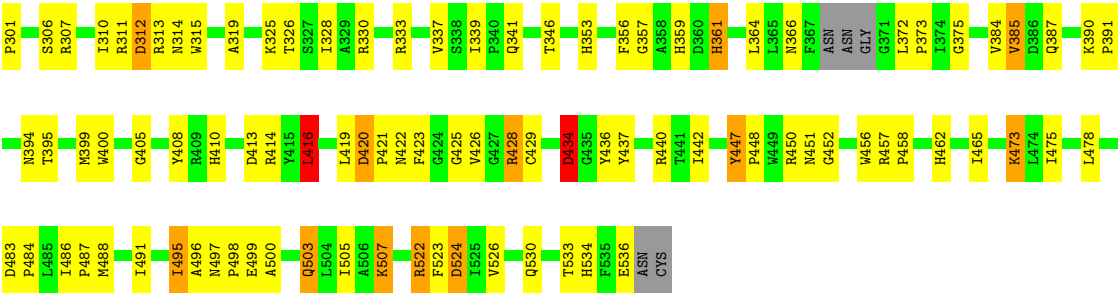
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain R:

58%

34%

5% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.39Å 126.52Å 133.33Å 90.00° 97.77° 90.00°	Depositor
Resolution (Å)	6.00 – 2.05	Depositor
% Data completeness (in resolution range)	75.2 (6.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22080	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CME, FE, CHB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.28	4/1611 (0.2%)	1.86	34/2195 (1.5%)
1	B	1.32	3/1611 (0.2%)	1.86	32/2195 (1.5%)
1	C	1.23	1/1611 (0.1%)	1.76	23/2195 (1.0%)
1	D	1.30	3/1611 (0.2%)	1.85	26/2195 (1.2%)
1	E	1.31	3/1611 (0.2%)	1.78	31/2195 (1.4%)
1	F	1.29	3/1611 (0.2%)	1.85	25/2195 (1.1%)
2	M	1.41	5/1888 (0.3%)	1.97	47/2569 (1.8%)
2	N	1.44	10/1888 (0.5%)	1.86	34/2569 (1.3%)
2	O	1.45	12/1888 (0.6%)	1.90	40/2569 (1.6%)
2	P	1.40	3/1888 (0.2%)	1.93	45/2569 (1.8%)
2	Q	1.46	10/1888 (0.5%)	1.94	46/2569 (1.8%)
2	R	1.39	4/1888 (0.2%)	1.97	46/2569 (1.8%)
All	All	1.37	61/20994 (0.3%)	1.88	429/28584 (1.5%)

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

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	9.02	1.56	1.52
2	R	428	ARG	CD-NE	-8.14	1.34	1.46
1	C	133	ARG	CA-C	7.81	1.62	1.52
2	M	428	ARG	CD-NE	-7.79	1.35	1.46
2	Q	428	ARG	CD-NE	-7.77	1.35	1.46
2	N	451	ASN	CA-C	7.68	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	486	ILE	CA-CB	7.60	1.57	1.54
1	B	94	ARG	CD-NE	-7.40	1.35	1.46
2	Q	461	ILE	CA-C	7.19	1.61	1.52
2	Q	441	THR	CA-CB	7.08	1.63	1.53
2	P	440	ARG	CD-NE	-7.06	1.36	1.46
2	Q	440	ARG	CD-NE	-6.89	1.36	1.46
2	N	440	ARG	CD-NE	-6.89	1.36	1.46
2	R	375	GLY	N-CA	6.87	1.52	1.45
2	Q	321	THR	N-CA	6.47	1.53	1.46
2	N	441	THR	CA-CB	6.34	1.62	1.53
1	A	94	ARG	CD-NE	-6.28	1.37	1.46
2	N	467	GLY	CA-C	6.25	1.60	1.51
1	D	108	THR	CA-CB	6.15	1.62	1.54
2	M	451	ASN	CA-C	6.11	1.56	1.52
2	N	428	ARG	CD-NE	-6.01	1.37	1.46
2	P	451	ASN	CA-C	5.99	1.55	1.52
2	M	379	ILE	CA-C	5.98	1.59	1.52
2	P	321	THR	CA-CB	5.89	1.61	1.53
2	Q	449	TRP	N-CA	5.86	1.53	1.45
1	E	94	ARG	CD-NE	-5.84	1.38	1.46
2	Q	452	GLY	N-CA	5.82	1.52	1.44
1	F	94	ARG	CD-NE	-5.82	1.38	1.46
2	O	379	ILE	CA-C	5.80	1.59	1.52
1	E	108	THR	CA-CB	5.76	1.61	1.53
1	E	133	ARG	CA-C	5.67	1.59	1.52
2	O	309	VAL	C-N	-5.61	1.27	1.33
2	O	509	ASP	N-CA	5.59	1.54	1.46
2	M	326	THR	CA-CB	5.58	1.62	1.53
2	N	326	THR	CB-OG1	5.56	1.52	1.43
2	O	475	ILE	C-O	5.52	1.29	1.24
2	O	441	THR	CA-CB	5.51	1.61	1.53
1	A	5	LEU	CA-C	5.48	1.59	1.53
1	D	4	LEU	N-CA	5.45	1.52	1.45
2	O	324	TYR	CA-C	5.43	1.59	1.53
1	A	8	THR	CA-CB	5.43	1.61	1.53
2	N	528	ARG	NE-CZ	5.42	1.39	1.33
2	O	428	ARG	CD-NE	-5.37	1.38	1.46
2	Q	375	GLY	N-CA	5.36	1.50	1.45
1	A	108	THR	CA-CB	5.31	1.60	1.53
2	M	441	THR	CA-CB	5.23	1.60	1.54
2	O	321	THR	CA-CB	5.21	1.60	1.53
1	B	133	ARG	CD-NE	-5.20	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	527	LEU	N-CA	5.13	1.51	1.45
2	N	343	ILE	CA-CB	5.13	1.60	1.54
1	F	36	TRP	CA-C	-5.10	1.48	1.53
2	Q	440	ARG	N-CA	5.08	1.52	1.46
2	Q	326	THR	CB-OG1	5.07	1.51	1.43
1	F	93	GLY	N-CA	5.07	1.50	1.45
1	D	130	LEU	C-O	5.06	1.30	1.24
2	R	495	ILE	CA-CB	5.05	1.60	1.54
2	O	533	THR	CB-OG1	5.04	1.51	1.43
1	B	108	THR	CA-CB	5.03	1.60	1.53
2	R	524	ASP	N-CA	5.01	1.51	1.45
2	N	382	GLY	N-CA	5.01	1.50	1.45
2	O	472	THR	CA-CB	5.00	1.61	1.53

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ARG	CD-NE-CZ	17.48	148.88	124.40
1	F	133	ARG	CD-NE-CZ	16.39	147.35	124.40
1	B	133	ARG	CD-NE-CZ	15.28	145.78	124.40
1	A	94	ARG	CD-NE-CZ	12.75	142.25	124.40
2	O	353	HIS	CA-CB-CG	-12.58	101.22	113.80
2	M	428	ARG	CD-NE-CZ	12.40	141.76	124.40
2	P	440	ARG	NE-CZ-NH2	-12.27	108.16	119.20
2	O	434	ASP	CA-CB-CG	-12.09	100.51	112.60
2	R	434	ASP	CA-CB-CG	-11.79	100.81	112.60
2	P	353	HIS	CA-CB-CG	-11.64	102.16	113.80
2	Q	451	ASN	O-C-N	11.34	129.22	120.83
2	O	428	ARG	CD-NE-CZ	11.18	140.04	124.40
2	M	434	ASP	CA-CB-CG	-11.16	101.44	112.60
2	R	428	ARG	CG-CD-NE	10.97	136.14	112.00
2	M	440	ARG	NE-CZ-NH2	-10.95	109.34	119.20
2	N	452	GLY	N-CA-C	-10.91	99.03	112.23
2	Q	452	GLY	N-CA-C	-10.79	99.17	112.23
2	Q	428	ARG	CD-NE-CZ	10.75	139.45	124.40
2	R	361	HIS	CA-CB-CG	-10.65	103.15	113.80
2	Q	440	ARG	NE-CZ-NH2	-10.61	109.65	119.20
2	N	451	ASN	O-C-N	10.43	128.55	120.83
2	R	353	HIS	CA-CB-CG	-10.26	103.54	113.80
2	Q	447	TYR	O-C-N	10.22	129.01	121.85
2	P	434	ASP	CA-CB-CG	-9.89	102.71	112.60
2	Q	394	ASN	CA-CB-CG	-9.77	102.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	452	GLY	N-CA-C	-9.61	100.61	112.23
1	B	184	ARG	NE-CZ-NH2	-9.58	110.57	119.20
1	D	94	ARG	NE-CZ-NH2	-9.51	110.64	119.20
2	N	440	ARG	NE-CZ-NH2	-9.42	110.72	119.20
2	O	452	GLY	N-CA-C	-9.37	100.89	112.23
2	O	440	ARG	NE-CZ-NH2	-9.37	110.77	119.20
2	R	452	GLY	N-CA-C	-9.21	101.09	112.23
2	Q	361	HIS	CA-CB-CG	-9.20	104.60	113.80
2	R	440	ARG	NE-CZ-NH2	-9.16	110.96	119.20
2	Q	428	ARG	CB-CG-CD	9.01	132.02	111.30
2	O	451	ASN	O-C-N	8.98	127.47	120.83
2	R	339	ILE	O-C-N	8.96	127.34	121.69
2	P	440	ARG	NE-CZ-NH1	8.91	130.41	121.50
2	P	361	HIS	CA-CB-CG	-8.87	104.93	113.80
2	M	452	GLY	N-CA-C	-8.71	101.69	112.23
2	Q	428	ARG	NE-CZ-NH2	-8.58	111.48	119.20
2	O	420	ASP	CB-CA-C	8.57	119.68	110.17
2	Q	514	ASN	O-C-N	8.51	129.19	121.19
1	F	107	HIS	CA-CB-CG	-8.40	105.40	113.80
1	D	19	ILE	CB-CA-C	8.36	123.42	112.14
2	O	447	TYR	O-C-N	8.28	127.65	121.85
2	O	361	HIS	CA-CB-CG	-8.13	105.67	113.80
1	A	99	PHE	CA-CB-CG	8.12	121.92	113.80
2	N	353	HIS	CA-CB-CG	-8.07	105.73	113.80
1	B	94	ARG	CG-CD-NE	8.01	129.63	112.00
1	F	19	ILE	CB-CA-C	7.97	122.90	112.14
1	A	21	LEU	N-CA-C	7.96	124.07	113.72
1	D	37	ASN	N-CA-C	7.95	122.56	113.02
2	Q	451	ASN	CA-C-O	-7.94	115.24	119.77
1	A	94	ARG	NE-CZ-NH1	7.93	129.43	121.50
2	M	428	ARG	CG-CD-NE	7.89	129.35	112.00
2	P	451	ASN	O-C-N	7.85	127.78	120.71
1	F	61	HIS	CA-CB-CG	-7.82	105.98	113.80
1	A	94	ARG	NE-CZ-NH2	-7.79	112.19	119.20
2	M	447	TYR	O-C-N	7.71	127.85	121.83
2	P	450	ARG	CD-NE-CZ	7.71	135.19	124.40
2	R	428	ARG	CB-CG-CD	7.67	128.94	111.30
2	R	428	ARG	CD-NE-CZ	7.65	135.12	124.40
2	M	353	HIS	CA-CB-CG	-7.61	106.19	113.80
2	O	440	ARG	O-C-N	7.61	132.21	123.31
1	E	37	ASN	N-CA-C	7.57	121.41	112.93
1	F	94	ARG	CB-CG-CD	7.57	128.70	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	326	THR	CA-CB-OG1	-7.51	98.33	109.60
1	C	87	ASN	CA-CB-CG	7.50	120.10	112.60
1	B	94	ARG	CB-CG-CD	7.47	128.48	111.30
2	R	394	ASN	CA-CB-CG	-7.46	105.14	112.60
1	A	19	ILE	CB-CA-C	7.46	122.22	112.14
1	E	94	ARG	CG-CD-NE	7.35	128.17	112.00
1	E	133	ARG	N-CA-C	-7.30	99.65	110.23
2	Q	333	ARG	CB-CA-C	7.30	121.33	109.07
1	C	47	GLU	CB-CG-CD	7.27	124.96	112.60
2	N	434	ASP	CA-CB-CG	-7.26	105.33	112.60
1	C	127	ASN	CA-CB-CG	-7.26	105.34	112.60
2	R	325	LYS	N-CA-C	7.25	120.10	111.33
1	A	37	ASN	N-CA-C	7.21	121.01	112.93
2	M	411	LYS	CB-CA-C	-7.21	98.77	110.74
1	B	76	ASN	CA-CB-CG	-7.21	105.39	112.60
2	P	440	ARG	CD-NE-CZ	7.21	134.49	124.40
2	N	514	ASN	O-C-N	7.20	127.95	121.19
1	A	5	LEU	N-CA-C	-7.15	100.75	109.83
1	E	99	PHE	CA-CB-CG	7.14	120.94	113.80
2	N	361	HIS	CA-CB-CG	-7.10	106.70	113.80
2	R	447	TYR	O-C-N	7.10	127.38	121.84
1	B	178	ASP	CB-CA-C	7.10	121.97	111.89
1	F	133	ARG	NE-CZ-NH2	7.06	125.55	119.20
1	E	76	ASN	CA-CB-CG	-7.02	105.58	112.60
1	F	94	ARG	CD-NE-CZ	7.01	134.22	124.40
2	P	359	HIS	CA-CB-CG	-6.99	106.81	113.80
1	C	37	ASN	N-CA-C	6.98	121.40	113.02
2	N	461	ILE	O-C-N	6.97	130.79	123.26
1	D	18	HIS	CA-CB-CG	-6.97	106.83	113.80
2	Q	461	ILE	O-C-N	6.97	130.79	123.26
1	F	37	ASN	N-CA-C	6.96	120.73	112.93
1	B	171	ILE	N-CA-C	6.88	117.76	107.51
1	A	167	ARG	CD-NE-CZ	-6.86	114.79	124.40
2	Q	428	ARG	CG-CD-NE	6.86	127.10	112.00
2	R	312	ASP	CA-CB-CG	-6.83	105.77	112.60
1	B	133	ARG	NE-CZ-NH1	6.82	128.32	121.50
2	M	494	SER	N-CA-C	-6.80	104.24	112.54
2	P	414	ARG	CD-NE-CZ	-6.78	114.91	124.40
2	R	440	ARG	NH1-CZ-NH2	6.78	128.11	119.30
2	O	326	THR	CA-CB-OG1	-6.75	99.48	109.60
2	O	451	ASN	CA-C-O	-6.73	115.94	119.77
1	E	52	LEU	CB-CA-C	6.68	122.39	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	451	ASN	CA-CB-CG	-6.68	105.92	112.60
1	A	47	GLU	CB-CG-CD	6.65	123.90	112.60
1	D	28	ASN	O-C-N	6.61	126.97	121.35
2	N	428	ARG	CB-CG-CD	6.60	126.48	111.30
2	M	339	ILE	O-C-N	6.59	125.84	121.69
2	O	304	ASP	CA-CB-CG	6.57	119.17	112.60
2	M	402	ALA	O-C-N	6.56	130.35	122.68
2	R	422	ASN	CA-CB-CG	-6.56	106.04	112.60
1	E	28	ASN	O-C-N	6.56	126.67	121.55
2	Q	499	GLU	CB-CG-CD	6.54	123.71	112.60
2	N	428	ARG	CG-CD-NE	6.53	126.38	112.00
1	B	133	ARG	NE-CZ-NH2	-6.53	113.32	119.20
2	N	326	THR	CA-CB-OG1	-6.49	99.86	109.60
1	B	176	GLU	CB-CG-CD	6.49	123.63	112.60
2	P	512	ASN	OD1-CG-ND2	6.47	129.07	122.60
2	Q	311	ARG	CD-NE-CZ	6.46	133.44	124.40
1	E	90	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	87	ASN	CA-CB-CG	6.45	119.05	112.60
2	Q	326	THR	CA-CB-OG1	-6.41	99.99	109.60
1	E	5	LEU	N-CA-C	-6.40	101.25	110.08
1	C	99	PHE	CA-CB-CG	6.39	120.19	113.80
2	N	451	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	A	5	LEU	O-C-N	6.38	128.58	121.43
2	M	451	ASN	OD1-CG-ND2	6.38	128.98	122.60
2	M	440	ARG	CB-CG-CD	-6.37	96.65	111.30
2	M	450	ARG	CD-NE-CZ	6.37	133.31	124.40
1	C	133	ARG	N-CA-C	-6.35	101.02	110.23
2	N	314	ASN	CA-CB-CG	-6.35	106.25	112.60
1	D	3	GLU	CB-CG-CD	6.34	123.38	112.60
1	B	71	TRP	CA-CB-CG	6.33	125.62	113.60
2	Q	314	ASN	CA-CB-CG	-6.32	106.28	112.60
2	P	367	PHE	CA-C-O	-6.31	110.07	120.80
1	F	43	ASP	CA-CB-CG	-6.31	106.29	112.60
2	P	314	ASN	CB-CA-C	6.29	120.75	109.29
2	P	512	ASN	CA-CB-CG	-6.29	106.31	112.60
2	O	440	ARG	CB-CG-CD	-6.29	96.84	111.30
1	A	30	THR	CA-CB-OG1	-6.28	100.18	109.60
2	Q	372	LEU	N-CA-CB	-6.28	99.75	110.11
2	O	387	GLN	OE1-CD-NE2	6.26	128.86	122.60
1	D	57	ASP	CA-C-N	6.26	127.96	120.14
1	D	57	ASP	C-N-CA	6.26	127.96	120.14
1	A	9	PRO	CB-CA-C	-6.25	102.90	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	494	SER	N-CA-C	-6.24	104.76	112.38
2	N	489	CYS	O-C-N	6.24	126.61	121.31
2	N	470	ILE	O-C-N	6.23	128.84	121.80
1	F	94	ARG	CG-CD-NE	6.22	125.68	112.00
1	B	117	ALA	CA-C-O	-6.20	113.97	120.55
1	B	5	LEU	N-CA-C	-6.18	101.98	109.83
1	B	94	ARG	CD-NE-CZ	6.17	133.04	124.40
2	R	458	PRO	CB-CA-C	-6.16	103.35	111.23
2	Q	495	ILE	O-C-N	6.15	129.39	122.68
2	Q	434	ASP	CA-CB-CG	-6.15	106.45	112.60
2	R	534	HIS	CA-CB-CG	6.15	119.95	113.80
1	C	158	LEU	CB-CA-C	6.12	120.96	110.79
2	N	348	GLY	O-C-N	6.09	127.86	121.77
1	F	5	LEU	N-CA-C	-6.09	102.09	109.83
2	O	428	ARG	NE-CZ-NH1	6.09	127.59	121.50
2	P	496	ALA	CA-C-N	6.08	129.77	121.74
2	P	496	ALA	C-N-CA	6.08	129.77	121.74
2	R	522	ARG	CD-NE-CZ	-6.07	115.90	124.40
2	P	428	ARG	NE-CZ-NH1	6.07	127.57	121.50
2	M	492	VAL	N-CA-C	-6.07	104.59	110.72
1	C	11	GLN	CA-C-O	-6.06	114.20	120.99
2	P	428	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	184	ARG	CD-NE-CZ	6.05	132.87	124.40
2	P	489	CYS	N-CA-C	6.05	118.38	109.42
1	E	14	GLY	CA-C-N	6.04	125.67	119.56
1	E	14	GLY	C-N-CA	6.04	125.67	119.56
1	F	171	ILE	N-CA-C	6.04	117.15	107.73
2	M	533	THR	CA-CB-OG1	-6.02	100.58	109.60
2	O	314	ASN	CB-CA-C	6.01	120.23	109.29
2	O	428	ARG	N-CA-CB	6.01	120.71	110.50
1	D	43	ASP	CA-CB-CG	-5.99	106.61	112.60
1	A	126	ILE	O-C-N	5.97	129.70	123.26
2	R	314	ASN	OD1-CG-ND2	5.97	128.57	122.60
1	B	59	ASN	CA-CB-CG	-5.96	106.64	112.60
1	C	19	ILE	CA-CB-CG2	5.93	120.58	110.50
1	D	126	ILE	O-C-N	5.92	129.66	123.26
1	A	115	ASN	CA-CB-CG	5.92	118.52	112.60
2	P	447	TYR	CA-CB-CG	-5.92	103.24	113.90
2	N	372	LEU	N-CA-CB	-5.92	100.34	110.11
2	O	314	ASN	N-CA-C	-5.92	106.22	113.50
2	Q	339	ILE	O-C-N	5.91	125.41	121.69
1	B	37	ASN	N-CA-C	5.91	120.11	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	465	ILE	O-C-N	5.90	129.31	123.18
2	R	428	ARG	NE-CZ-NH2	-5.89	113.90	119.20
2	O	492	VAL	N-CA-C	-5.89	104.77	110.42
1	D	5	LEU	N-CA-C	-5.88	102.36	109.83
1	E	165	GLN	CB-CG-CD	5.87	122.59	112.60
2	M	417	ALA	N-CA-C	-5.87	102.37	109.83
2	M	459	ALA	N-CA-C	-5.85	101.74	110.23
2	Q	449	TRP	CB-CA-C	5.84	122.54	109.56
2	N	316	HIS	CA-CB-CG	-5.84	107.96	113.80
2	M	383	ARG	CD-NE-CZ	-5.83	116.23	124.40
1	A	3	GLU	CB-CG-CD	5.83	122.51	112.60
2	O	514	ASN	O-C-N	5.83	126.67	121.19
2	M	361	HIS	CA-CB-CG	-5.80	108.00	113.80
2	N	350	ASN	CA-CB-CG	-5.79	106.81	112.60
2	P	428	ARG	CD-NE-CZ	5.79	132.50	124.40
1	D	178	ASP	CA-CB-CG	-5.79	106.81	112.60
1	B	186	ASP	O-C-N	5.77	129.52	123.06
2	Q	463	PHE	O-C-N	5.76	130.33	123.24
1	E	186	ASP	O-C-N	5.76	129.73	123.10
1	C	171	ILE	N-CA-C	5.76	116.09	107.51
1	A	138	HIS	CA-CB-CG	-5.75	108.05	113.80
2	P	326	THR	CA-CB-OG1	-5.75	100.97	109.60
2	P	314	ASN	N-CA-C	-5.75	106.43	113.50
1	D	159	ASN	CA-CB-CG	-5.75	106.85	112.60
1	A	155	CYS	O-C-N	5.74	126.52	121.18
2	Q	446	PRO	N-CA-C	-5.74	103.18	111.22
2	Q	489	CYS	O-C-N	5.74	126.63	121.35
2	M	440	ARG	NH1-CZ-NH2	5.73	126.75	119.30
2	M	328	ILE	N-CA-C	5.73	115.86	110.30
1	D	133	ARG	NE-CZ-NH1	5.72	127.22	121.50
2	Q	458	PRO	CB-CA-C	-5.72	103.74	111.12
1	A	177	VAL	O-C-N	5.71	129.11	123.18
1	E	107	HIS	CA-CB-CG	-5.71	108.09	113.80
2	M	372	LEU	CB-CA-C	5.70	116.61	108.68
2	R	333	ARG	N-CA-C	-5.70	106.68	113.97
2	N	447	TYR	CA-CB-CG	-5.69	103.65	113.90
2	Q	440	ARG	CB-CG-CD	-5.69	98.21	111.30
2	R	387	GLN	OE1-CD-NE2	5.69	128.29	122.60
2	N	387	GLN	OE1-CD-NE2	5.69	128.29	122.60
2	M	314	ASN	CA-CB-CG	-5.69	106.91	112.60
2	O	316	HIS	O-C-N	5.68	127.62	121.60
2	P	514	ASN	OD1-CG-ND2	-5.68	116.92	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	494	SER	N-CA-C	-5.66	105.47	112.38
2	M	392	VAL	O-C-N	5.65	127.54	121.10
1	D	163	GLN	O-C-N	5.64	125.80	121.23
2	M	333	ARG	CB-CA-C	5.63	118.53	109.07
2	N	333	ARG	N-CA-C	-5.63	106.96	113.88
1	F	76	ASN	CA-CB-CG	-5.62	106.98	112.60
2	M	394	ASN	CB-CG-ND2	5.62	124.83	116.40
2	O	379	ILE	N-CA-C	-5.62	100.39	108.53
1	C	5	LEU	O-C-N	5.61	127.72	121.43
2	O	451	ASN	N-CA-C	-5.60	99.56	108.30
1	E	36	TRP	CB-CA-C	5.58	121.53	110.42
1	C	187	ILE	O-C-N	5.58	129.04	123.18
2	P	385	VAL	CA-C-O	-5.58	115.81	121.67
2	R	457	ARG	CD-NE-CZ	5.58	132.21	124.40
2	N	357	GLY	CA-C-N	5.58	128.02	120.38
2	N	357	GLY	C-N-CA	5.58	128.02	120.38
2	R	385	VAL	O-C-N	5.56	129.12	123.00
1	B	28	ASN	O-C-N	5.56	126.20	121.20
2	P	447	TYR	CB-CA-C	5.55	117.47	109.92
1	E	88	ALA	N-CA-C	-5.55	105.24	112.23
1	C	150	GLN	N-CA-CB	5.55	118.06	110.01
1	F	18	HIS	CA-CB-CG	-5.54	108.26	113.80
2	M	403	ASN	O-C-N	5.54	129.00	121.74
1	D	94	ARG	CB-CG-CD	5.54	124.04	111.30
1	F	21	LEU	N-CA-CB	-5.54	102.55	110.80
2	M	443	LYS	CG-CD-CE	5.53	124.02	111.30
1	B	8	THR	CA-C-O	5.53	124.95	119.75
1	B	86	GLU	CB-CG-CD	5.53	122.00	112.60
2	R	440	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	A	8	THR	CA-C-N	5.53	125.29	119.76
1	A	8	THR	C-N-CA	5.53	125.29	119.76
2	Q	346	THR	CA-CB-OG1	-5.53	101.31	109.60
2	N	357	GLY	N-CA-C	-5.52	105.48	112.54
1	A	94	ARG	CG-CD-NE	5.52	124.14	112.00
1	F	162	GLU	CA-CB-CG	5.51	125.13	114.10
1	F	162	GLU	N-CA-CB	5.51	118.19	109.82
2	O	372	LEU	N-CA-C	-5.51	102.00	110.32
2	O	416	LEU	CB-CA-C	5.51	121.82	110.31
1	E	43	ASP	CA-CB-CG	-5.50	107.11	112.60
2	R	419	LEU	N-CA-C	-5.50	103.13	110.55
2	N	440	ARG	CB-CG-CD	-5.49	98.69	111.30
1	F	52	LEU	CB-CA-C	5.48	120.82	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	333	ARG	N-CA-C	-5.48	106.96	113.97
1	E	38	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	A	19	ILE	CA-CB-CG1	5.47	119.70	110.40
2	Q	458	PRO	N-CA-C	-5.47	102.85	111.34
2	M	450	ARG	NE-CZ-NH1	5.47	126.97	121.50
2	P	494	SER	N-CA-C	-5.46	105.71	112.38
2	P	497	ASN	CA-C-N	5.46	125.81	119.47
2	P	497	ASN	C-N-CA	5.46	125.81	119.47
2	O	359	HIS	CA-CB-CG	-5.46	108.34	113.80
2	R	357	GLY	CA-C-N	5.46	127.59	120.28
2	R	357	GLY	C-N-CA	5.46	127.59	120.28
1	B	94	ARG	NE-CZ-NH1	5.45	126.95	121.50
2	Q	419	LEU	N-CA-C	-5.45	102.42	110.48
2	Q	428	ARG	N-CA-CB	5.44	119.74	110.50
2	P	386	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	171	ILE	N-CA-C	5.43	116.54	108.23
1	B	136	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	A	166	ARG	CD-NE-CZ	5.43	132.00	124.40
2	M	458	PRO	CB-CA-C	-5.42	104.13	111.12
2	P	366	ASN	N-CA-C	5.42	119.64	113.19
2	P	432	ASP	O-C-N	5.41	128.83	121.74
1	A	18	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	106	LEU	N-CA-CB	-5.41	101.34	111.13
1	D	19	ILE	CA-CB-CG1	5.41	119.59	110.40
1	C	183	TYR	N-CA-CB	5.40	119.89	110.81
2	Q	372	LEU	N-CA-C	-5.40	102.86	110.31
2	P	446	PRO	N-CA-C	-5.39	103.67	111.22
2	R	533	THR	CA-CB-OG1	-5.38	101.54	109.60
1	C	5	LEU	N-CA-C	-5.36	102.38	109.84
1	D	152	ASN	OD1-CG-ND2	5.36	127.96	122.60
2	N	449	TRP	CB-CA-C	5.36	121.36	109.94
1	E	8	THR	CA-C-N	5.35	125.11	119.76
1	E	8	THR	C-N-CA	5.35	125.11	119.76
1	A	41	LYS	N-CA-C	-5.34	103.20	110.36
2	Q	529	GLY	N-CA-C	-5.34	105.11	111.36
2	Q	471	ALA	O-C-N	5.34	128.84	122.27
2	Q	481	GLU	CB-CG-CD	5.33	121.67	112.60
2	R	473	LYS	CG-CD-CE	5.32	123.54	111.30
2	P	442	ILE	CB-CA-C	5.31	118.53	110.62
1	B	177	VAL	O-C-N	5.31	128.18	123.03
1	E	94	ARG	NE-CZ-NH1	5.31	126.81	121.50
2	O	394	ASN	CA-CB-CG	-5.30	107.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	CD-NE-CZ	5.30	131.82	124.40
2	R	375	GLY	N-CA-C	-5.30	106.23	111.85
2	N	439	PHE	O-C-N	5.30	129.42	123.27
1	F	140	HIS	CB-CA-C	-5.30	101.00	109.75
2	M	333	ARG	N-CA-C	-5.29	107.19	113.97
2	M	535	PHE	CA-C-O	-5.29	115.40	121.54
2	R	496	ALA	N-CA-C	5.29	117.13	111.36
2	R	311	ARG	N-CA-CB	5.29	117.78	110.17
2	P	422	ASN	CA-CB-CG	-5.28	107.32	112.60
2	Q	350	ASN	CB-CA-C	5.26	118.90	110.16
1	F	5	LEU	O-C-N	5.26	127.33	121.43
2	R	457	ARG	O-C-N	5.26	127.33	121.43
1	A	196	VAL	O-C-N	5.26	128.35	122.61
1	E	189	ILE	O-C-N	5.26	126.97	121.87
1	A	90	ASN	CA-CB-CG	5.25	117.85	112.60
1	B	149	ALA	O-C-N	5.25	128.15	122.11
2	Q	524	ASP	O-C-N	5.25	128.94	123.06
2	M	497	ASN	CA-C-N	5.25	125.30	119.32
2	M	497	ASN	C-N-CA	5.25	125.30	119.32
2	N	308	PHE	CB-CA-C	5.24	118.81	109.38
2	R	483	ASP	O-C-N	5.24	125.86	121.31
1	A	43	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	69	GLU	N-CA-CB	5.23	119.47	110.68
1	E	112	GLY	N-CA-C	-5.23	104.43	112.85
1	D	8	THR	OG1-CB-CG2	5.22	119.75	109.30
1	E	48	HIS	CA-CB-CG	-5.22	108.58	113.80
2	Q	440	ARG	NH1-CZ-NH2	5.20	126.07	119.30
2	M	496	ALA	N-CA-C	5.20	116.95	111.28
2	Q	348	GLY	O-C-N	5.20	126.97	121.77
2	R	420	ASP	O-C-N	5.18	127.03	121.12
1	C	11	GLN	N-CA-CB	5.18	121.15	111.52
1	F	90	ASN	CB-CA-C	5.18	119.19	109.71
1	D	66	SER	CB-CA-C	5.17	118.97	109.46
1	D	139	LEU	CB-CA-C	5.17	118.16	109.48
1	A	131	PHE	CA-CB-CG	5.17	118.97	113.80
2	R	491	ILE	N-CA-CB	5.16	117.17	110.57
1	B	4	LEU	N-CA-CB	-5.16	102.60	110.49
1	A	60	GLY	N-CA-C	-5.15	108.16	115.43
2	N	533	THR	CA-CB-OG1	-5.15	101.87	109.60
1	A	165	GLN	OE1-CD-NE2	-5.15	117.45	122.60
1	C	36	TRP	N-CA-C	5.14	115.17	108.07
2	P	479	TYR	CA-C-O	-5.14	115.45	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	448	PRO	O-C-N	5.14	129.38	123.06
2	M	427	GLY	CA-C-N	5.13	130.94	121.70
2	M	427	GLY	C-N-CA	5.13	130.94	121.70
2	M	518	CYS	O-C-N	5.13	129.10	123.25
2	R	451	ASN	O-C-N	5.13	129.42	122.59
2	M	432	ASP	CA-C-N	5.13	127.41	120.38
2	M	432	ASP	C-N-CA	5.13	127.41	120.38
1	E	61	HIS	CA-CB-CG	-5.13	108.67	113.80
1	E	178	ASP	N-CA-C	-5.13	104.34	111.52
2	R	416	LEU	CB-CA-C	5.13	121.14	110.32
1	E	133	ARG	O-C-N	5.12	129.17	122.87
1	D	116	ASN	N-CA-C	-5.12	103.92	110.53
1	F	7	GLU	CB-CG-CD	5.12	121.31	112.60
2	R	394	ASN	O-C-N	5.12	129.11	122.40
2	P	514	ASN	O-C-N	5.12	126.96	121.12
2	Q	499	GLU	CG-CD-OE1	5.12	130.18	118.40
2	R	434	ASP	OD1-CG-OD2	5.12	135.19	122.90
1	B	41	LYS	N-CA-C	-5.12	103.22	110.29
2	M	532	LYS	N-CA-C	-5.12	103.64	110.55
1	B	184	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	B	38	ARG	CD-NE-CZ	5.12	131.56	124.40
1	F	166	ARG	CD-NE-CZ	5.12	131.56	124.40
2	P	514	ASN	CA-CB-CG	5.11	117.71	112.60
2	O	533	THR	CA-CB-OG1	-5.11	101.93	109.60
2	Q	380	VAL	O-C-N	5.11	128.46	122.99
1	F	106	LEU	N-CA-CB	-5.11	101.88	111.13
1	E	51	LEU	CA-C-O	-5.10	115.30	120.71
2	M	411	LYS	CA-CB-CG	5.10	124.30	114.10
2	M	507	LYS	O-C-N	5.09	129.15	123.19
2	Q	526	VAL	O-C-N	5.09	128.60	123.20
2	P	529	GLY	N-CA-C	-5.09	105.40	111.36
2	N	386	ASP	CA-CB-CG	5.09	117.69	112.60
2	R	394	ASN	OD1-CG-ND2	5.09	127.69	122.60
2	O	372	LEU	CB-CA-C	5.09	115.73	108.76
1	D	196	VAL	O-C-N	5.09	128.21	122.67
2	P	457	ARG	CA-CB-CG	5.09	124.27	114.10
1	E	125	HIS	CA-CB-CG	-5.09	108.71	113.80
2	Q	372	LEU	CB-CA-C	5.08	115.75	108.68
1	C	100	ASP	CA-C-N	5.08	127.60	120.28
1	C	100	ASP	C-N-CA	5.08	127.60	120.28
2	O	339	ILE	O-C-N	5.08	126.89	121.10
2	P	529	GLY	CA-C-O	5.08	125.88	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	415	TYR	CB-CA-C	5.08	118.34	109.65
2	R	319	ALA	O-C-N	5.08	127.58	122.09
2	N	312	ASP	CA-CB-CG	-5.08	107.52	112.60
1	F	38	ARG	CA-CB-CG	5.07	124.25	114.10
2	O	353	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	C	159	ASN	CA-CB-CG	-5.07	107.53	112.60
1	C	136	ASN	O-C-N	5.06	127.92	122.15
2	O	321	THR	N-CA-CB	-5.06	104.82	111.09
2	M	385	VAL	O-C-N	5.05	128.56	122.95
1	B	38	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	E	37	ASN	CA-CB-CG	-5.05	107.55	112.60
2	O	400	TRP	N-CA-CB	5.05	120.92	111.52
2	R	357	GLY	N-CA-C	-5.05	105.85	112.82
2	P	324	TYR	N-CA-C	-5.05	98.49	107.98
1	C	131	PHE	CA-CB-CG	5.04	118.84	113.80
2	R	384	VAL	O-C-N	5.04	129.00	123.10
2	P	392	VAL	O-C-N	5.04	126.84	121.10
1	D	150	GLN	O-C-N	5.03	127.52	122.09
2	O	504	LEU	CA-C-N	-5.03	116.47	122.90
2	O	504	LEU	C-N-CA	-5.03	116.47	122.90
1	B	115	ASN	O-C-N	5.02	128.87	123.10
2	N	451	ASN	N-CA-C	-5.01	100.48	108.30
2	P	322	PRO	CB-CA-C	5.01	120.63	112.26
2	Q	358	ALA	CA-C-O	-5.01	115.24	120.55
2	O	320	LEU	CB-CA-C	5.00	119.06	110.81
1	E	41	LYS	N-CA-C	-5.00	103.39	110.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain

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	1571	0	1499	62	0
1	B	1571	0	1499	56	0
1	C	1571	0	1499	60	0
1	D	1571	0	1499	60	0
1	E	1571	0	1499	68	0
1	F	1571	0	1499	81	0
2	M	1844	0	1796	81	0
2	N	1844	0	1796	41	0
2	O	1844	0	1796	61	0
2	P	1844	0	1796	68	0
2	Q	1844	0	1796	64	0
2	R	1844	0	1796	60	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	22	0	7	1	0
4	N	22	0	7	2	0
4	O	22	0	6	2	0
4	P	22	0	7	0	0
4	Q	22	0	7	2	0
4	R	22	0	7	2	0
5	A	82	0	0	3	0
5	B	83	0	0	4	0
5	C	84	0	0	4	0
5	D	84	0	0	2	0
5	E	83	0	0	3	0
5	F	83	0	0	3	0
5	M	160	0	0	4	0
5	N	164	0	0	2	0
5	O	155	0	0	6	0
5	P	153	0	0	4	0
5	Q	163	0	0	4	0
5	R	158	0	0	2	0
All	All	22080	0	19811	690	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 17.

All (690) 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)
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.16	1.14
1:E:165:GLN:H	1:E:165:GLN:NE2	1.47	1.11
1:B:18:HIS:ND1	5:B:648:HOH:O	1.83	1.09
1:F:165:GLN:H	1:F:165:GLN:NE2	1.52	1.07
1:D:18:HIS:ND1	5:D:648:HOH:O	1.88	1.07
1:B:165:GLN:H	1:B:165:GLN:NE2	1.52	1.06
1:C:133:ARG:HD2	2:O:326:THR:HG21	1.33	1.05
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.22	1.02
1:E:165:GLN:HE21	1:E:165:GLN:N	1.56	1.02
1:F:18:HIS:ND1	5:F:648:HOH:O	1.93	0.99
1:C:18:HIS:ND1	5:C:648:HOH:O	1.74	0.97
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.79	0.96
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.29	0.96
1:E:18:HIS:ND1	5:E:648:HOH:O	1.99	0.95
1:F:64:ARG:NH1	1:F:100:ASP:O	2.03	0.91
1:C:165:GLN:H	1:C:165:GLN:NE2	1.67	0.90
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.54	0.89
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.86	0.89
2:R:361:HIS:H	2:R:361:HIS:CD2	1.86	0.89
1:E:78:GLU:OE1	5:E:692:HOH:O	1.91	0.87
2:R:361:HIS:H	2:R:361:HIS:HD2	1.22	0.86
1:A:69:GLU:OE1	2:M:473:LYS:HE2	1.75	0.85
1:C:134:GLY:HA3	2:O:326:THR:HG22	1.60	0.84
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.06	0.83
2:O:390:LYS:HD3	5:O:677:HOH:O	1.78	0.83
1:D:64:ARG:NH1	1:D:100:ASP:O	2.12	0.83
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.61	0.82
1:F:49:ILE:HA	1:F:180:LYS:HE3	1.61	0.82
2:P:390:LYS:HE2	5:P:756:HOH:O	1.78	0.82
1:C:133:ARG:CD	2:O:326:THR:HG21	2.10	0.81
1:C:177:VAL:O	1:C:180:LYS:HB3	1.79	0.81
2:Q:361:HIS:CD2	2:Q:361:HIS:H	1.98	0.81
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.15	0.81
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.62	0.81
2:M:390:LYS:HD2	5:M:642:HOH:O	1.80	0.81
1:B:165:GLN:NE2	1:B:165:GLN:N	2.27	0.80
2:P:361:HIS:H	2:P:361:HIS:CD2	2.00	0.80
1:F:98:THR:OG1	1:F:102:GLY:N	2.14	0.80
1:B:176:GLU:HG3	1:B:180:LYS:O	1.81	0.79
1:C:133:ARG:HG3	1:C:133:ARG:O	1.71	0.78
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.45	0.77
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:H	1:B:165:GLN:CD	1.92	0.77
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.50	0.76
1:B:176:GLU:HG3	1:B:180:LYS:C	2.10	0.76
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.68	0.76
1:F:165:GLN:NE2	1:F:165:GLN:N	2.32	0.76
1:F:165:GLN:H	1:F:165:GLN:CD	1.94	0.75
1:D:165:GLN:NE2	1:D:165:GLN:H	1.82	0.75
1:E:131:PHE:CE1	1:E:138:HIS:HB3	2.22	0.75
1:C:98:THR:OG1	1:C:102:GLY:N	2.21	0.74
1:D:177:VAL:O	1:D:180:LYS:HB3	1.88	0.74
2:P:361:HIS:H	2:P:361:HIS:HD2	1.34	0.73
2:N:478:LEU:C	2:N:478:LEU:HD23	2.12	0.73
1:C:133:ARG:HD2	2:O:326:THR:CG2	2.15	0.73
1:F:50:LEU:HD12	1:F:51:LEU:N	2.04	0.72
1:F:165:GLN:H	1:F:165:GLN:HE21	1.37	0.72
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.71	0.72
1:C:64:ARG:NH1	1:C:100:ASP:O	2.22	0.72
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.38	0.71
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.54	0.71
2:M:497:ASN:ND2	2:M:499:GLU:H	1.87	0.71
1:B:3:GLU:HA	1:B:3:GLU:OE1	1.90	0.71
2:O:361:HIS:H	2:O:361:HIS:CD2	2.09	0.71
1:B:98:THR:O	1:B:102:GLY:HA2	1.90	0.71
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.71	0.71
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.71	0.71
1:C:165:GLN:H	1:C:165:GLN:HE21	1.37	0.71
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.91	0.70
2:P:497:ASN:C	2:P:497:ASN:HD22	1.99	0.70
2:R:497:ASN:HD22	2:R:499:GLU:H	1.38	0.69
1:A:98:THR:HB	1:A:100:ASP:OD1	1.91	0.69
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.39	0.69
1:A:134:GLY:CA	2:M:326:THR:HG22	2.23	0.69
2:N:361:HIS:CD2	2:N:361:HIS:H	2.11	0.69
1:E:99:PHE:HE2	2:Q:411:LYS:HE3	1.57	0.69
2:M:361:HIS:H	2:M:361:HIS:CD2	2.10	0.69
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.59	0.68
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.74	0.68
2:R:497:ASN:ND2	2:R:499:GLU:H	1.91	0.68
2:M:497:ASN:HD22	2:M:498:PRO:N	1.92	0.68
1:A:165:GLN:CD	1:A:165:GLN:H	2.02	0.68
1:A:18:HIS:NE2	5:A:648:HOH:O	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.76	0.67
1:D:114:VAL:HG23	1:D:122:MET:HE3	1.77	0.67
1:E:99:PHE:CE2	2:Q:411:LYS:HE3	2.29	0.67
2:R:361:HIS:CD2	2:R:361:HIS:N	2.58	0.67
2:N:497:ASN:HD22	2:N:499:GLU:H	1.43	0.67
2:Q:390:LYS:HD2	5:Q:670:HOH:O	1.95	0.66
2:O:497:ASN:HD22	2:O:499:GLU:H	1.41	0.66
1:B:49:ILE:HA	1:B:180:LYS:HE2	1.77	0.66
2:P:497:ASN:ND2	2:P:499:GLU:H	1.93	0.66
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.11	0.66
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.60	0.66
2:O:411:LYS:HG2	2:O:412:ASN:ND2	2.10	0.66
1:D:19:ILE:O	2:P:426:VAL:HG21	1.96	0.65
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.96	0.65
1:B:163:GLN:CB	1:B:165:GLN:HE22	2.04	0.65
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.11	0.65
1:B:144:TYR:CE1	1:B:158:LEU:HD13	2.31	0.65
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.12	0.65
1:E:131:PHE:CD1	1:E:138:HIS:HB3	2.31	0.65
1:F:143:LEU:C	1:F:143:LEU:HD23	2.20	0.65
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.62	0.65
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.96	0.65
1:A:100:ASP:OD1	1:A:100:ASP:N	2.27	0.65
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.61	0.65
2:Q:505:ILE:O	2:Q:507:LYS:HE3	1.97	0.65
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.78	0.65
2:N:356:PHE:HD2	2:N:428:ARG:HD3	1.61	0.64
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.33	0.64
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.45	0.64
1:D:165:GLN:H	1:D:165:GLN:HE21	1.44	0.64
2:Q:447:TYR:HE2	4:Q:550:CHB:H5	1.62	0.64
1:F:165:GLN:N	1:F:165:GLN:HE21	1.95	0.64
2:O:408:TYR:HE2	2:O:447:TYR:CZ	2.17	0.63
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.13	0.63
2:O:447:TYR:HE2	4:O:550:CHB:H5	1.64	0.63
1:F:100:ASP:CG	1:F:101:ALA:H	2.06	0.63
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.33	0.63
2:O:390:LYS:HE2	5:O:800:HOH:O	1.98	0.63
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.12	0.63
2:M:497:ASN:HD22	2:M:497:ASN:C	2.07	0.63
2:R:447:TYR:CE1	4:R:550:CHB:H5	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.80	0.62
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.34	0.62
1:E:98:THR:OG1	1:E:102:GLY:N	2.30	0.62
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.35	0.62
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.34	0.62
1:C:19:ILE:HG13	2:O:426:VAL:HG22	1.82	0.62
2:O:361:HIS:CG	2:O:429:CME:HE3	2.34	0.62
1:D:110:LYS:NZ	1:D:147:ASP:OD1	2.30	0.62
2:N:453:PRO:HB2	2:O:310:ILE:HD12	1.81	0.62
1:E:98:THR:HB	1:E:100:ASP:OD1	1.99	0.62
1:F:114:VAL:HG23	1:F:122:MET:HE3	1.81	0.62
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.82	0.62
2:N:448:PRO:HD3	2:N:456:TRP:CZ3	2.35	0.62
2:R:447:TYR:HE1	4:R:550:CHB:H5	1.65	0.62
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.81	0.61
1:D:100:ASP:CG	1:D:101:ALA:H	2.07	0.61
1:F:98:THR:O	1:F:102:GLY:HA2	2.00	0.61
1:E:165:GLN:H	1:E:165:GLN:HE21	0.72	0.61
2:Q:390:LYS:HD3	5:Q:748:HOH:O	1.99	0.61
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.82	0.61
1:C:44:ALA:O	1:C:48:HIS:NE2	2.28	0.61
1:E:143:LEU:HD23	1:E:143:LEU:C	2.25	0.61
1:A:78:GLU:OE1	2:M:301:PRO:HB3	2.01	0.61
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.26	0.61
1:A:64:ARG:NH1	1:A:100:ASP:O	2.33	0.60
2:P:405:GLY:HA3	5:P:686:HOH:O	2.00	0.60
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.26	0.60
1:D:180:LYS:HG3	1:D:181:THR:N	2.14	0.60
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.01	0.60
2:M:364:LEU:HB2	2:M:440:ARG:HD3	1.83	0.60
2:N:497:ASN:ND2	2:N:499:GLU:H	1.99	0.60
2:O:497:ASN:ND2	2:O:499:GLU:H	2.00	0.60
1:F:98:THR:HB	1:F:100:ASP:OD1	2.01	0.60
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.16	0.60
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.84	0.60
1:E:100:ASP:CG	1:E:101:ALA:H	2.09	0.60
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.36	0.60
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.65	0.60
1:C:143:LEU:HD23	1:C:143:LEU:C	2.27	0.60
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.02	0.60
2:R:405:GLY:HA3	5:R:682:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.82	0.59
2:Q:408:TYR:HE2	2:Q:447:TYR:CZ	2.20	0.59
1:C:52:LEU:C	1:C:52:LEU:HD22	2.27	0.59
2:P:442:ILE:C	2:P:442:ILE:HD12	2.27	0.59
2:P:448:PRO:HD3	2:P:456:TRP:CZ3	2.38	0.59
2:O:416:LEU:C	2:O:416:LEU:HD23	2.26	0.59
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.84	0.59
1:D:99:PHE:HE2	2:P:411:LYS:HE3	1.68	0.59
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.18	0.59
1:E:177:VAL:O	1:E:180:LYS:HB3	2.02	0.59
1:A:176:GLU:HA	1:A:180:LYS:O	2.03	0.59
2:N:522:ARG:NH1	5:N:762:HOH:O	2.29	0.58
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.84	0.58
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.84	0.58
1:B:165:GLN:N	1:B:165:GLN:HE21	2.01	0.58
2:N:447:TYR:HB2	2:N:448:PRO:HD2	1.86	0.58
1:B:52:LEU:C	1:B:52:LEU:HD22	2.29	0.58
2:O:486:ILE:N	2:O:487:PRO:HD2	2.19	0.58
1:B:18:HIS:CG	5:B:648:HOH:O	2.43	0.57
1:F:19:ILE:HG21	2:R:410:HIS:HB2	1.85	0.57
2:O:361:HIS:H	2:O:361:HIS:HD2	1.53	0.57
1:F:18:HIS:CG	5:F:648:HOH:O	2.50	0.57
2:M:361:HIS:H	2:M:361:HIS:HD2	1.52	0.57
1:A:133:ARG:HG3	2:M:326:THR:HG21	1.86	0.57
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.39	0.57
2:N:361:HIS:H	2:N:361:HIS:HD2	1.49	0.57
2:O:376:GLU:O	2:O:442:ILE:HA	2.04	0.57
2:P:484:PRO:O	2:P:488:MET:HE3	2.05	0.57
1:F:19:ILE:HD11	2:R:408:TYR:HD2	1.70	0.57
2:P:497:ASN:HD22	2:P:499:GLU:H	1.51	0.57
1:F:80:GLN:O	1:F:91:SER:HB2	2.04	0.57
2:Q:361:HIS:CG	2:Q:429:CME:HE3	2.40	0.57
2:R:408:TYR:HE1	2:R:447:TYR:CZ	2.23	0.57
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.40	0.57
1:D:51:LEU:O	1:D:105:THR:HA	2.05	0.57
1:C:176:GLU:HG2	1:C:179:GLY:HA2	1.85	0.56
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.20	0.56
1:D:176:GLU:HA	1:D:180:LYS:O	2.05	0.56
2:Q:447:TYR:HB2	2:Q:448:PRO:HD2	1.86	0.56
1:C:98:THR:O	1:C:102:GLY:HA2	2.05	0.56
1:F:177:VAL:O	1:F:180:LYS:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:447:TYR:HB2	2:M:448:PRO:HD2	1.88	0.56
1:C:98:THR:HB	1:C:100:ASP:OD1	2.04	0.56
1:C:100:ASP:CG	1:C:101:ALA:H	2.13	0.56
1:E:164:PRO:HD2	1:E:165:GLN:HE22	1.70	0.56
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.21	0.56
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	1.87	0.56
2:R:447:TYR:HB2	2:R:448:PRO:HD2	1.87	0.56
2:M:408:TYR:HE2	2:M:447:TYR:CZ	2.23	0.56
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.87	0.56
1:A:155:CYS:HB3	1:A:158:LEU:HB2	1.86	0.56
2:P:416:LEU:C	2:P:416:LEU:HD23	2.30	0.56
2:P:478:LEU:C	2:P:478:LEU:HD23	2.31	0.56
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.06	0.56
1:E:52:LEU:HD23	1:E:103:GLU:CD	2.31	0.55
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.88	0.55
2:O:447:TYR:CE2	4:O:550:CHB:H5	2.41	0.55
2:P:307:ARG:CG	2:P:533:THR:HG22	2.34	0.55
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.21	0.55
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.36	0.55
1:A:100:ASP:CG	1:A:101:ALA:H	2.13	0.55
1:E:98:THR:O	1:E:102:GLY:HA2	2.06	0.55
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.14	0.55
1:A:176:GLU:HG3	1:A:180:LYS:N	2.21	0.55
2:M:448:PRO:HB2	2:P:516:MET:HA	1.89	0.55
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.88	0.55
1:D:155:CYS:HB3	1:D:158:LEU:HB2	1.88	0.55
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.88	0.55
1:B:64:ARG:NH1	1:B:100:ASP:O	2.40	0.54
2:P:390:LYS:HD3	5:P:683:HOH:O	2.07	0.54
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.70	0.54
1:D:98:THR:HB	1:D:100:ASP:OD1	2.08	0.54
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.39	0.54
1:B:176:GLU:OE2	1:B:179:GLY:O	2.24	0.54
2:P:408:TYR:HE2	2:P:447:TYR:CZ	2.26	0.54
2:R:400:TRP:HA	2:R:425:GLY:O	2.08	0.54
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.53	0.54
2:N:447:TYR:CE1	2:N:460:HIS:HE1	2.26	0.54
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.08	0.54
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.41	0.54
2:R:484:PRO:O	2:R:488:MET:HE3	2.07	0.54
1:C:36:TRP:CG	1:C:37:ASN:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.90	0.53
1:B:140:HIS:O	1:B:197:PHE:HA	2.08	0.53
1:B:143:LEU:C	1:B:143:LEU:HD23	2.32	0.53
2:O:316:HIS:HB3	2:O:317:PRO:HD2	1.90	0.53
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.08	0.53
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.72	0.53
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.41	0.53
2:N:416:LEU:HD23	2:N:416:LEU:C	2.32	0.53
2:P:497:ASN:HD22	2:P:498:PRO:N	2.06	0.53
1:C:100:ASP:OD1	1:C:100:ASP:N	2.42	0.53
2:Q:447:TYR:CE1	2:Q:460:HIS:HE1	2.26	0.53
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.44	0.53
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.91	0.53
2:R:522:ARG:NH1	5:R:716:HOH:O	2.40	0.53
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.91	0.52
1:B:33:GLN:CG	1:B:85:LEU:HD12	2.39	0.52
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.90	0.52
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.34	0.52
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.42	0.52
1:D:143:LEU:C	1:D:143:LEU:HD23	2.35	0.52
1:F:176:GLU:HA	1:F:180:LYS:O	2.09	0.52
2:N:359:HIS:O	2:N:366:ASN:HB3	2.09	0.52
1:C:84:ASN:OD1	1:C:86:GLU:HB2	2.09	0.52
1:D:98:THR:O	1:D:102:GLY:HA2	2.08	0.52
1:F:36:TRP:CG	1:F:37:ASN:H	2.28	0.52
2:O:486:ILE:N	2:O:487:PRO:CD	2.73	0.52
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.24	0.52
2:R:437:TYR:CD1	2:R:437:TYR:C	2.87	0.52
2:R:505:ILE:HG22	2:R:507:LYS:HE2	1.91	0.52
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.92	0.52
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.40	0.52
1:F:131:PHE:O	1:F:132:ALA:HB2	2.10	0.52
1:B:50:LEU:O	1:B:182:ALA:HA	2.10	0.52
2:O:373:PRO:HB3	2:O:423:PHE:HB2	1.90	0.52
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.91	0.52
1:A:51:LEU:HD12	1:A:106:LEU:HD23	1.91	0.51
2:N:315:TRP:HZ2	2:N:503:GLN:NE2	2.08	0.51
1:D:54:GLN:HG3	1:D:184:ARG:NH2	2.25	0.51
2:M:416:LEU:C	2:M:416:LEU:HD23	2.35	0.51
1:E:144:TYR:CE1	1:E:158:LEU:HD13	2.45	0.51
2:P:376:GLU:O	2:P:442:ILE:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.91	0.51
2:Q:326:THR:HG22	2:Q:330:ARG:HD2	1.91	0.51
1:F:100:ASP:OD1	1:F:100:ASP:N	2.40	0.51
1:D:52:LEU:C	1:D:52:LEU:HD22	2.35	0.51
1:D:165:GLN:HE21	1:D:165:GLN:N	2.09	0.51
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.46	0.51
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.76	0.51
2:P:359:HIS:O	2:P:366:ASN:HB3	2.11	0.51
2:M:376:GLU:O	2:M:442:ILE:HA	2.11	0.51
2:P:326:THR:CG2	2:P:330:ARG:HD2	2.41	0.51
1:E:165:GLN:NE2	1:E:165:GLN:N	2.33	0.51
1:C:18:HIS:HA	1:C:22:ALA:HB3	1.93	0.51
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.41	0.51
2:O:308:PHE:CE2	2:O:530:GLN:HB2	2.45	0.51
2:M:383:ARG:HD2	2:M:436:TYR:CZ	2.46	0.51
1:D:99:PHE:CE2	2:P:411:LYS:HE3	2.44	0.51
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	1.92	0.51
1:C:28:ASN:HB3	5:C:817:HOH:O	2.10	0.51
1:D:16:TYR:O	1:D:19:ILE:HG23	2.11	0.51
1:D:98:THR:OG1	1:D:102:GLY:N	2.40	0.51
2:M:495:ILE:HG21	2:M:500:ALA:HB3	1.93	0.50
2:P:447:TYR:HB2	2:P:448:PRO:HD2	1.92	0.50
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.92	0.50
1:F:38:ARG:HA	1:F:107:HIS:HB2	1.93	0.50
2:R:497:ASN:HD22	2:R:497:ASN:C	2.20	0.50
2:N:497:ASN:HD22	2:N:497:ASN:C	2.18	0.50
1:C:19:ILE:O	2:O:426:VAL:HG21	2.11	0.50
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.45	0.50
2:P:442:ILE:HD12	2:P:442:ILE:O	2.11	0.50
1:E:161:ILE:O	1:E:167:ARG:NH2	2.44	0.50
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.11	0.50
2:R:522:ARG:HE	2:R:524:ASP:CG	2.20	0.50
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.50
2:P:400:TRP:HA	2:P:425:GLY:O	2.12	0.50
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.09	0.50
1:F:44:ALA:O	1:F:48:HIS:NE2	2.31	0.50
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.94	0.50
2:R:416:LEU:C	2:R:416:LEU:HD23	2.37	0.50
2:M:505:ILE:HG22	2:M:507:LYS:HE2	1.94	0.50
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.42	0.50
1:D:36:TRP:CG	1:D:37:ASN:H	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.27	0.49
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.93	0.49
2:N:376:GLU:O	2:N:442:ILE:HA	2.12	0.49
2:O:408:TYR:CE2	2:O:447:TYR:CZ	3.00	0.49
1:E:35:ILE:HG21	1:E:92:PHE:HE1	1.76	0.49
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.94	0.49
1:A:28:ASN:HB3	5:A:817:HOH:O	2.12	0.49
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.95	0.49
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.93	0.49
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.49
1:A:78:GLU:HG2	2:M:301:PRO:HG3	1.94	0.49
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.47	0.49
1:B:165:GLN:N	1:B:165:GLN:CD	2.67	0.49
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.47	0.49
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.93	0.49
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.95	0.49
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.94	0.49
2:N:447:TYR:HE2	4:N:550:CHB:H5	1.78	0.49
1:C:19:ILE:HG12	2:O:400:TRP:HB2	1.93	0.49
1:D:18:HIS:CG	5:D:648:HOH:O	2.48	0.49
2:P:414:ARG:NE	2:P:414:ARG:HA	2.28	0.49
2:Q:405:GLY:HA3	5:Q:673:HOH:O	2.13	0.49
1:F:36:TRP:CD1	1:F:37:ASN:H	2.31	0.49
2:P:325:LYS:HG2	2:Q:335:ALA:HB1	1.94	0.49
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.13	0.49
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.95	0.49
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.95	0.49
2:N:447:TYR:CE2	4:N:550:CHB:H5	2.48	0.48
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.42	0.48
1:E:131:PHE:O	1:E:132:ALA:HB2	2.12	0.48
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.12	0.48
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.42	0.48
1:A:50:LEU:O	1:A:182:ALA:HA	2.13	0.48
1:A:98:THR:O	1:A:102:GLY:HA2	2.13	0.48
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.95	0.48
2:M:361:HIS:CG	2:M:429:CME:HE3	2.48	0.48
1:E:36:TRP:CG	1:E:37:ASN:H	2.32	0.48
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.13	0.48
2:M:478:LEU:HD23	2:M:478:LEU:C	2.37	0.48
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.95	0.48
1:F:176:GLU:HG3	1:F:180:LYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG3	1:A:180:LYS:O	2.13	0.48
2:M:318:LYS:HD3	2:M:318:LYS:HA	1.50	0.48
1:B:98:THR:HB	1:B:100:ASP:OD1	2.14	0.48
2:O:484:PRO:O	2:O:488:MET:HE3	2.13	0.48
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.96	0.48
2:N:360:ASP:OD2	2:N:428:ARG:HD2	2.14	0.48
2:O:364:LEU:HB2	2:O:440:ARG:HD3	1.96	0.48
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.95	0.48
2:P:411:LYS:O	2:P:414:ARG:NH1	2.46	0.48
2:P:437:TYR:CD1	2:P:437:TYR:C	2.92	0.48
2:P:489:CYS:HB3	2:P:492:VAL:HB	1.96	0.48
1:E:61:HIS:CE1	1:F:163:GLN:HG3	2.49	0.48
1:E:64:ARG:NH1	1:E:100:ASP:O	2.45	0.48
1:E:131:PHE:CE1	1:E:138:HIS:CB	2.95	0.48
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.48	0.48
1:C:165:GLN:HE21	1:C:165:GLN:N	2.07	0.48
2:O:447:TYR:CE1	2:O:460:HIS:HE1	2.32	0.48
1:D:54:GLN:HG3	1:D:184:ARG:HH22	1.79	0.48
1:E:52:LEU:O	1:E:184:ARG:HA	2.14	0.48
1:F:50:LEU:O	1:F:182:ALA:HA	2.14	0.48
1:A:52:LEU:O	1:A:184:ARG:HA	2.14	0.47
1:A:180:LYS:HG3	1:A:181:THR:N	2.29	0.47
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.79	0.47
1:B:176:GLU:HA	1:B:180:LYS:O	2.12	0.47
2:P:473:LYS:HD2	2:P:474:LEU:N	2.29	0.47
2:Q:429:CME:HE2	2:Q:438:SER:O	2.14	0.47
2:M:522:ARG:NH1	5:M:666:HOH:O	2.31	0.47
1:D:134:GLY:HA3	2:P:326:THR:CG2	2.40	0.47
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.75	0.47
1:E:114:VAL:HG23	1:E:122:MET:CE	2.44	0.47
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.96	0.47
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.29	0.47
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.50	0.47
2:O:403:ASN:HB2	5:O:620:HOH:O	2.15	0.47
1:D:191:GLY:O	1:D:194:GLU:HB2	2.13	0.47
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.50	0.47
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.96	0.47
2:M:516:MET:HB3	2:M:516:MET:HE3	1.60	0.47
1:F:49:ILE:CA	1:F:180:LYS:HE3	2.38	0.47
2:M:497:ASN:ND2	2:M:497:ASN:C	2.72	0.47
1:C:165:GLN:H	1:C:165:GLN:CD	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:356:PHE:HD2	2:P:428:ARG:HD3	1.79	0.47
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.95	0.47
2:Q:447:TYR:CE2	4:Q:550:CHB:H5	2.46	0.47
2:R:359:HIS:O	2:R:366:ASN:HB3	2.15	0.47
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.80	0.47
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.45	0.47
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.15	0.47
1:F:50:LEU:HD12	1:F:50:LEU:C	2.38	0.47
1:F:69:GLU:OE2	1:F:94:ARG:HD3	2.15	0.47
2:M:399:MET:HA	2:M:462:HIS:O	2.15	0.47
2:M:465:ILE:HG12	2:M:525:ILE:HD13	1.96	0.47
1:E:140:HIS:O	1:E:197:PHE:HA	2.14	0.47
2:M:473:LYS:NZ	5:M:652:HOH:O	2.48	0.46
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.97	0.46
2:O:413:ASP:C	2:O:414:ARG:HD2	2.40	0.46
2:Q:447:TYR:OH	2:Q:460:HIS:CE1	2.67	0.46
2:Q:488:MET:CE	1:F:1:PRO:HG2	2.45	0.46
2:R:306:SER:CB	2:R:530:GLN:HE21	2.28	0.46
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.96	0.46
1:E:176:GLU:HA	1:E:180:LYS:O	2.16	0.46
2:M:381:ALA:O	2:M:522:ARG:HA	2.15	0.46
2:P:392:VAL:HG12	2:P:395:THR:HB	1.95	0.46
2:Q:447:TYR:CE1	2:Q:460:HIS:CE1	3.03	0.46
2:M:429:CME:HE2	2:M:438:SER:O	2.15	0.46
2:M:448:PRO:CB	2:P:516:MET:HA	2.46	0.46
1:B:74:ASP:HB2	5:B:690:HOH:O	2.16	0.46
1:B:180:LYS:HD2	1:B:181:THR:H	1.81	0.46
2:Q:465:ILE:HD12	2:Q:465:ILE:N	2.29	0.46
1:A:36:TRP:CG	1:A:37:ASN:H	2.32	0.46
2:M:361:HIS:CD2	2:M:361:HIS:N	2.81	0.46
1:C:11:GLN:HB2	2:O:477:GLN:HG3	1.97	0.46
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.80	0.46
1:F:114:VAL:HG23	1:F:122:MET:CE	2.45	0.46
2:R:341:GLN:HB3	2:R:346:THR:CG2	2.46	0.46
2:N:414:ARG:NE	2:N:414:ARG:HA	2.30	0.46
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.16	0.46
2:M:519:LEU:HD21	2:P:456:TRP:CG	2.50	0.46
1:D:165:GLN:H	1:D:165:GLN:CD	2.24	0.46
2:P:484:PRO:O	2:P:487:PRO:HD2	2.16	0.46
1:E:51:LEU:HD12	1:E:106:LEU:CD2	2.45	0.46
2:M:386:ASP:HA	2:M:527:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:505:ILE:O	2:R:507:LYS:HE3	2.16	0.46
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.78	0.45
1:E:50:LEU:O	1:E:182:ALA:HA	2.16	0.45
2:P:489:CYS:C	2:P:493:LYS:HE3	2.41	0.45
1:F:162:GLU:O	1:F:164:PRO:HD3	2.15	0.45
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.64	0.45
2:M:361:HIS:ND1	2:M:429:CME:HE3	2.32	0.45
2:M:385:VAL:O	2:M:526:VAL:HA	2.16	0.45
1:B:180:LYS:HD2	1:B:181:THR:N	2.31	0.45
2:R:385:VAL:O	2:R:526:VAL:HA	2.15	0.45
1:D:39:LEU:HB3	1:D:90:ASN:O	2.17	0.45
2:R:408:TYR:HE1	2:R:447:TYR:CE2	2.34	0.45
2:M:516:MET:HA	2:P:448:PRO:HB2	1.98	0.45
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.52	0.45
1:D:15:PRO:HB3	1:D:133:ARG:HD3	1.99	0.45
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.99	0.45
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.47	0.45
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.31	0.45
2:N:381:ALA:O	2:N:522:ARG:HA	2.17	0.45
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.51	0.45
1:F:77:GLY:O	1:F:114:VAL:HG12	2.16	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.81	0.45
2:P:443:LYS:HE2	2:P:480:PHE:CG	2.52	0.45
1:E:180:LYS:HD2	1:E:181:THR:O	2.17	0.45
2:R:413:ASP:C	2:R:414:ARG:HD2	2.42	0.45
1:A:19:ILE:HD11	2:M:408:TYR:HD1	1.81	0.45
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.99	0.45
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.98	0.45
1:D:164:PRO:O	1:D:167:ARG:HB2	2.17	0.45
2:Q:522:ARG:HD3	5:Q:694:HOH:O	2.16	0.45
2:O:361:HIS:CD2	5:O:866:HOH:O	2.70	0.44
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.47	0.44
1:F:176:GLU:OE2	1:F:179:GLY:C	2.60	0.44
2:M:515:PRO:HB3	2:P:453:PRO:O	2.17	0.44
1:D:176:GLU:CG	1:D:179:GLY:HA2	2.48	0.44
2:P:360:ASP:O	2:P:427:GLY:HA2	2.18	0.44
1:E:51:LEU:HB2	1:E:106:LEU:HB3	2.00	0.44
2:Q:408:TYR:CE2	2:Q:447:TYR:CZ	3.04	0.44
1:F:50:LEU:HD12	1:F:51:LEU:H	1.79	0.44
2:R:373:PRO:HB3	2:R:423:PHE:HB2	2.00	0.44
1:B:36:TRP:CG	1:B:37:ASN:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:VAL:HG12	1:D:66:SER:HB3	1.98	0.44
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.32	0.44
2:P:381:ALA:O	2:P:522:ARG:HA	2.17	0.44
2:M:488:MET:HE2	1:B:1:PRO:HG2	1.98	0.44
1:B:114:VAL:HG23	1:B:122:MET:CE	2.48	0.44
2:O:313:ARG:O	2:O:318:LYS:HE2	2.17	0.44
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.17	0.44
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.99	0.44
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.82	0.44
1:E:44:ALA:O	1:E:48:HIS:NE2	2.32	0.44
1:F:174:ARG:HE	1:F:181:THR:HG23	1.83	0.44
1:B:28:ASN:HB3	5:B:817:HOH:O	2.17	0.44
1:D:84:ASN:OD1	1:D:86:GLU:HB2	2.18	0.44
2:P:373:PRO:HB3	2:P:423:PHE:HB2	1.99	0.44
1:F:57:ASP:OD1	1:F:59:ASN:N	2.48	0.44
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.47	0.44
2:M:447:TYR:CE1	2:M:460:HIS:HE1	2.36	0.44
2:M:497:ASN:HD22	2:M:498:PRO:CD	2.31	0.44
1:C:110:LYS:NZ	1:C:147:ASP:OD1	2.49	0.44
2:O:484:PRO:O	2:O:487:PRO:HD2	2.18	0.44
2:P:356:PHE:CD2	2:P:428:ARG:HD3	2.52	0.44
2:Q:486:ILE:N	2:Q:487:PRO:HD2	2.33	0.44
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.48	0.44
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.98	0.44
1:E:22:ALA:O	1:E:25:ALA:HB3	2.18	0.44
1:F:155:CYS:HB3	1:F:158:LEU:HB2	2.00	0.44
1:C:134:GLY:CA	2:O:326:THR:HG22	2.41	0.43
1:C:180:LYS:HD2	1:C:181:THR:N	2.33	0.43
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.52	0.43
2:M:400:TRP:HA	2:M:425:GLY:O	2.18	0.43
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.66	0.43
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.53	0.43
1:B:19:ILE:O	2:N:426:VAL:HG21	2.17	0.43
2:O:415:TYR:CE1	2:O:416:LEU:HD22	2.52	0.43
1:D:172:ALA:HB1	1:D:183:TYR:HB3	1.99	0.43
1:D:200:PHE:C	2:P:528:ARG:HH22	2.27	0.43
2:P:484:PRO:O	2:P:488:MET:CE	2.66	0.43
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.77	0.43
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.72	0.43
1:F:184:ARG:NH1	1:F:184:ARG:HG3	2.33	0.43
1:C:19:ILE:HG21	1:C:19:ILE:HD13	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:497:ASN:HD22	2:O:497:ASN:C	2.27	0.43
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.46	0.43
2:P:335:ALA:HB2	2:R:328:ILE:HD12	2.01	0.43
2:P:341:GLN:HB3	2:P:346:THR:CG2	2.49	0.43
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.43	0.43
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.66	0.43
2:R:486:ILE:N	2:R:487:PRO:HD2	2.33	0.43
2:N:405:GLY:HA3	5:N:742:HOH:O	2.18	0.43
1:F:30:THR:HB	1:F:34:GLU:HG3	2.01	0.43
1:F:199:ASP:CG	2:R:313:ARG:HE	2.26	0.43
1:A:12:THR:HA	1:A:135:ILE:O	2.18	0.43
1:A:54:GLN:HG3	1:A:184:ARG:HH22	1.83	0.43
1:C:176:GLU:HG2	1:C:179:GLY:CA	2.49	0.43
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.53	0.43
2:R:505:ILE:HG22	2:R:507:LYS:CE	2.48	0.43
1:A:41:LYS:O	1:A:48:HIS:HE1	2.02	0.43
1:B:64:ARG:HD3	1:B:99:PHE:O	2.18	0.43
2:N:478:LEU:C	2:N:478:LEU:CD2	2.85	0.43
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.54	0.43
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.77	0.43
1:D:116:ASN:OD1	1:D:116:ASN:C	2.60	0.43
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.88	0.43
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.92	0.43
2:M:400:TRP:CZ2	2:M:462:HIS:HB3	2.53	0.43
2:P:307:ARG:HD2	5:P:695:HOH:O	2.19	0.43
1:A:54:GLN:HG3	1:A:184:ARG:NH2	2.34	0.42
1:D:19:ILE:HG21	1:D:19:ILE:HD13	1.53	0.42
2:Q:447:TYR:CZ	2:Q:460:HIS:HE1	2.37	0.42
1:F:32:ASP:HB2	5:F:820:HOH:O	2.19	0.42
1:F:114:VAL:CG2	1:F:122:MET:HE3	2.47	0.42
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.49	0.42
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.92	0.42
1:C:19:ILE:O	2:O:426:VAL:CG2	2.67	0.42
1:E:18:HIS:CG	5:E:648:HOH:O	2.60	0.42
1:E:113:VAL:HG13	1:E:122:MET:O	2.19	0.42
2:R:450:ARG:HH11	2:R:450:ARG:HD2	1.65	0.42
1:A:165:GLN:NE2	1:A:165:GLN:H	2.17	0.42
1:B:12:THR:HA	1:B:135:ILE:O	2.20	0.42
2:N:484:PRO:O	2:N:488:MET:HE3	2.20	0.42
2:O:409:ARG:HD3	5:O:864:HOH:O	2.20	0.42
1:A:143:LEU:HD12	1:A:185:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.89	0.42
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.79	0.42
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.85	0.42
2:Q:399:MET:HA	2:Q:462:HIS:O	2.19	0.42
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.71	0.42
1:D:4:LEU:HB3	2:P:387:GLN:HB3	2.01	0.42
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.00	0.42
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.20	0.42
1:B:58:GLY:CA	1:B:190:GLN:HB3	2.49	0.42
1:C:18:HIS:CD2	1:C:22:ALA:HB3	2.55	0.42
1:C:39:LEU:HD11	1:C:93:GLY:HA3	2.02	0.42
1:C:180:LYS:HD2	1:C:181:THR:H	1.85	0.42
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.35	0.42
1:D:18:HIS:HD2	1:D:22:ALA:HB3	1.85	0.42
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	2.02	0.42
1:F:198:PHE:HA	2:R:337:VAL:O	2.20	0.42
2:M:497:ASN:HD22	2:M:499:GLU:H	1.63	0.42
2:M:505:ILE:O	2:M:507:LYS:HE3	2.20	0.42
1:B:114:VAL:CG2	1:B:122:MET:HE3	2.50	0.42
2:N:333:ARG:HD3	2:N:333:ARG:HA	1.99	0.42
1:D:176:GLU:HG3	1:D:179:GLY:HA2	2.02	0.42
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.55	0.42
2:R:434:ASP:HB3	2:R:436:TYR:CE2	2.55	0.42
2:M:307:ARG:NE	2:M:536:GLU:OE2	2.48	0.42
2:N:315:TRP:CZ2	2:N:503:GLN:NE2	2.85	0.42
2:O:437:TYR:CD1	2:O:437:TYR:C	2.97	0.42
2:P:443:LYS:HE2	2:P:480:PHE:CD2	2.55	0.42
2:R:312:ASP:C	2:R:312:ASP:OD1	2.63	0.42
2:R:399:MET:HA	2:R:462:HIS:O	2.19	0.42
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.88	0.41
1:C:176:GLU:CG	1:C:179:GLY:HA2	2.48	0.41
2:O:381:ALA:O	2:O:522:ARG:HA	2.20	0.41
2:Q:363:LEU:N	2:Q:363:LEU:HD12	2.35	0.41
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.17	0.41
1:F:52:LEU:HA	1:F:104:TRP:O	2.20	0.41
1:A:168:GLU:HA	1:A:171:ILE:HD12	2.00	0.41
1:E:35:ILE:HG21	1:E:92:PHE:CE1	2.54	0.41
1:F:19:ILE:O	2:R:426:VAL:HG21	2.20	0.41
1:F:158:LEU:HA	1:F:158:LEU:HD12	1.75	0.41
1:F:176:GLU:HG3	1:F:180:LYS:H	1.84	0.41
1:F:177:VAL:N	1:F:180:LYS:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:CG1	2:O:400:TRP:HB2	2.49	0.41
1:C:123:ALA:HB3	1:C:144:TYR:CE2	2.55	0.41
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.90	0.41
2:R:478:LEU:C	2:R:478:LEU:HD23	2.44	0.41
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.77	0.41
1:A:52:LEU:C	1:A:52:LEU:HD22	2.46	0.41
4:M:550:CHB:C4	5:M:742:HOH:O	2.68	0.41
1:D:132:ALA:HB3	1:D:135:ILE:HD12	2.01	0.41
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.88	0.41
1:B:100:ASP:OD1	1:B:100:ASP:N	2.49	0.41
5:C:697:HOH:O	2:O:426:VAL:HG21	2.20	0.41
2:O:326:THR:CG2	2:O:330:ARG:HD2	2.50	0.41
2:P:447:TYR:CE2	2:P:460:HIS:HE1	2.38	0.41
2:Q:350:ASN:OD1	2:Q:350:ASN:C	2.63	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.90	0.41
1:A:147:ASP:OD2	1:A:174:ARG:HD2	2.21	0.41
2:M:404:ALA:HB2	2:M:442:ILE:HD13	2.02	0.41
1:C:4:LEU:HB3	2:O:387:GLN:HB3	2.03	0.41
1:E:5:LEU:O	2:Q:387:GLN:HG2	2.20	0.41
2:R:364:LEU:CD1	2:R:442:ILE:HG23	2.50	0.41
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.55	0.41
1:A:18:HIS:CE1	1:A:99:PHE:CE1	3.09	0.41
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.46	0.41
1:B:176:GLU:OE2	1:B:179:GLY:C	2.64	0.41
2:N:486:ILE:N	2:N:487:PRO:HD2	2.36	0.41
1:C:51:LEU:HB2	1:C:106:LEU:HB3	2.02	0.41
1:A:18:HIS:CE1	5:A:648:HOH:O	2.70	0.41
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.16	0.41
2:M:359:HIS:O	2:M:366:ASN:HB3	2.21	0.41
2:M:413:ASP:C	2:M:414:ARG:HD2	2.46	0.41
2:O:399:MET:HA	2:O:462:HIS:O	2.20	0.41
1:D:36:TRP:HA	1:D:36:TRP:CE3	2.56	0.41
1:E:33:GLN:HG2	1:E:85:LEU:HD12	2.03	0.41
2:Q:321:THR:HG21	2:Q:494:SER:HB2	2.03	0.41
2:Q:378:ILE:O	2:Q:378:ILE:HG13	2.21	0.41
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.85	0.41
1:F:180:LYS:HD2	1:F:181:THR:H	1.85	0.41
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.51	0.41
1:C:18:HIS:HD2	1:C:22:ALA:HB3	1.86	0.41
1:C:50:LEU:O	1:C:182:ALA:HA	2.21	0.41
2:O:390:LYS:CE	5:O:800:HOH:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:HIS:CD2	1:D:22:ALA:HB3	2.56	0.41
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.56	0.41
1:E:51:LEU:HD11	1:E:126:ILE:HD12	2.02	0.41
2:R:361:HIS:CG	2:R:429:CME:HE3	2.56	0.41
1:A:84:ASN:OD1	1:A:86:GLU:HB2	2.21	0.40
1:C:18:HIS:CG	5:C:648:HOH:O	2.51	0.40
1:E:61:HIS:CG	1:F:163:GLN:HG3	2.55	0.40
1:E:65:ASP:OD2	1:E:133:ARG:NH1	2.45	0.40
1:E:84:ASN:OD1	1:E:86:GLU:HB2	2.22	0.40
1:F:19:ILE:HG22	1:F:26:ALA:HB1	2.03	0.40
1:B:36:TRP:CE3	1:B:36:TRP:HA	2.56	0.40
2:O:361:HIS:CD2	2:O:361:HIS:N	2.81	0.40
1:D:70:VAL:HG12	1:D:128:ILE:HG12	2.03	0.40
1:D:100:ASP:CG	1:D:101:ALA:N	2.78	0.40
2:Q:386:ASP:C	2:Q:386:ASP:OD1	2.63	0.40
1:F:180:LYS:HD2	1:F:181:THR:N	2.36	0.40
1:A:33:GLN:HG2	1:A:85:LEU:HD12	2.02	0.40
2:M:400:TRP:CE2	2:M:462:HIS:CB	3.05	0.40
2:M:431:THR:HA	2:M:436:TYR:O	2.21	0.40
1:B:78:GLU:HB3	2:N:301:PRO:HB3	2.02	0.40
1:C:114:VAL:CG2	1:C:122:MET:HE3	2.50	0.40
1:A:155:CYS:O	1:A:159:ASN:ND2	2.30	0.40
1:E:33:GLN:OE1	2:Q:354:LEU:HD12	2.21	0.40
2:Q:394:ASN:HD22	2:Q:394:ASN:HA	1.61	0.40
1:F:18:HIS:ND1	1:F:99:PHE:HZ	2.19	0.40
1:F:36:TRP:CG	1:F:37:ASN:N	2.90	0.40
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.89	0.40
2:M:392:VAL:HG12	2:M:395:THR:HB	2.04	0.40
2:O:385:VAL:O	2:O:526:VAL:HA	2.21	0.40
2:P:390:LYS:HA	2:P:391:PRO:HD3	1.98	0.40
1:E:110:LYS:HE2	1:E:148:GLU:OE2	2.22	0.40
2:Q:312:ASP:OD1	2:Q:312:ASP:C	2.64	0.40
2:R:420:ASP:HA	2:R:421:PRO:HD2	1.84	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	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	C	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	D	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	E	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	M	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
2	N	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	O	228/238 (96%)	218 (96%)	10 (4%)	0	100	100
2	P	228/238 (96%)	222 (97%)	6 (3%)	0	100	100
2	Q	228/238 (96%)	221 (97%)	7 (3%)	0	100	100
2	R	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
All	All	2556/2628 (97%)	2474 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	162/163 (99%)	155 (96%)	7 (4%)	26	20
1	B	162/163 (99%)	151 (93%)	11 (7%)	14	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	20
1	D	162/163 (99%)	156 (96%)	6 (4%)	30	25
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	25
1	F	162/163 (99%)	156 (96%)	6 (4%)	30	25
2	M	195/201 (97%)	185 (95%)	10 (5%)	21	14
2	N	195/201 (97%)	187 (96%)	8 (4%)	27	21
2	O	195/201 (97%)	187 (96%)	8 (4%)	27	21
2	P	195/201 (97%)	189 (97%)	6 (3%)	35	30
2	Q	195/201 (97%)	189 (97%)	6 (3%)	35	30
2	R	195/201 (97%)	188 (96%)	7 (4%)	31	26
All	All	2142/2184 (98%)	2054 (96%)	88 (4%)	27	21

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	52	LEU
1	A	94	ARG
1	A	158	LEU
1	A	165	GLN
1	A	192	GLU
2	M	301	PRO
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	434	ASP
2	M	440	ARG
2	M	473	LYS
2	M	478	LEU
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	38	ARG
1	B	50	LEU
1	B	52	LEU

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Mol	Chain	Res	Type
1	B	106	LEU
1	B	143	LEU
1	B	165	GLN
1	B	176	GLU
1	B	180	LYS
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	416	LEU
2	N	433	SER
2	N	478	LEU
2	N	499	GLU
2	N	507	LYS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	133	ARG
1	C	158	LEU
1	C	165	GLN
2	O	372	LEU
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	442	ILE
2	O	503	GLN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	52	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	372	LEU
2	P	395	THR
2	P	399	MET
2	P	414	ARG
2	P	416	LEU
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE

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Mol	Chain	Res	Type
1	E	32	ASP
1	E	52	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	301	PRO
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	143	LEU
1	F	165	GLN
1	F	180	LYS
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	434	ASP
2	R	473	LYS
2	R	503	GLN
2	R	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	165	GLN
2	M	359	HIS
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	11	GLN
1	B	165	GLN
2	N	334	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	127	ASN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	165	GLN
2	O	314	ASN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	59	ASN
1	D	163	GLN
1	D	165	GLN
2	P	334	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
1	E	163	GLN
1	E	165	GLN
2	Q	305	ASN
2	Q	334	GLN
2	Q	361	HIS
2	Q	394	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	534	HIS
1	F	11	GLN
1	F	59	ASN
1	F	127	ASN
1	F	165	GLN
2	R	353	HIS
2	R	359	HIS
2	R	361	HIS
2	R	412	ASN
2	R	497	ASN
2	R	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CME	Q	429	2	8,9,10	0.71	0	6,9,11	1.01	0
2	CME	M	429	2	8,9,10	0.89	0	6,9,11	0.47	0
2	CME	P	429	2	8,9,10	0.75	0	6,9,11	1.53	1 (16%)
2	CME	R	429	2	8,9,10	0.96	0	6,9,11	1.30	0
2	CME	N	429	2	8,9,10	0.75	0	6,9,11	1.20	1 (16%)
2	CME	O	429	2	8,9,10	0.53	0	6,9,11	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CME	Q	429	2	-	1/5/8/10	-
2	CME	M	429	2	-	0/5/8/10	-
2	CME	P	429	2	-	1/5/8/10	-
2	CME	R	429	2	-	0/5/8/10	-
2	CME	N	429	2	-	1/5/8/10	-
2	CME	O	429	2	-	2/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	429	CME	CZ-CE-SD	-2.72	104.28	113.39
2	N	429	CME	CB-SG-SD	2.43	110.14	103.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	429	CME	CZ-CE-SD-SG
2	O	429	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
2	N	429	CME	CZ-CE-SD-SG
2	O	429	CME	CZ-CE-SD-SG
2	P	429	CME	CZ-CE-SD-SG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	429	CME	2	0
2	M	429	CME	3	0
2	R	429	CME	1	0
2	O	429	CME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	CHB	R	551	-	11,11,11	1.17	1 (9%)	15,15,15	0.98	1 (6%)
4	CHB	M	551	-	11,11,11	1.15	2 (18%)	15,15,15	1.07	1 (6%)
4	CHB	N	551	-	11,11,11	1.25	1 (9%)	15,15,15	1.31	2 (13%)
4	CHB	N	550	3	11,11,11	1.06	1 (9%)	15,15,15	1.03	1 (6%)
4	CHB	P	551	-	11,11,11	1.31	2 (18%)	15,15,15	1.00	1 (6%)
4	CHB	M	550	3	11,11,11	1.13	1 (9%)	15,15,15	0.88	0
4	CHB	O	550	3	11,11,11	1.20	2 (18%)	15,15,15	1.13	1 (6%)
4	CHB	O	551	-	11,11,11	1.26	2 (18%)	15,15,15	1.19	2 (13%)
4	CHB	R	550	3	11,11,11	1.16	1 (9%)	15,15,15	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHB	P	550	3	11,11,11	1.35	2 (18%)	15,15,15	1.03	0
4	CHB	Q	550	3	11,11,11	1.22	2 (18%)	15,15,15	1.17	2 (13%)
4	CHB	Q	551	-	11,11,11	1.29	2 (18%)	15,15,15	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHB	R	551	-	-	0/4/4/4	0/1/1/1
4	CHB	M	551	-	-	0/4/4/4	0/1/1/1
4	CHB	N	551	-	-	0/4/4/4	0/1/1/1
4	CHB	N	550	3	-	0/4/4/4	0/1/1/1
4	CHB	P	551	-	-	0/4/4/4	0/1/1/1
4	CHB	M	550	3	-	0/4/4/4	0/1/1/1
4	CHB	O	550	3	-	0/4/4/4	0/1/1/1
4	CHB	O	551	-	-	0/4/4/4	0/1/1/1
4	CHB	R	550	3	-	0/4/4/4	0/1/1/1
4	CHB	P	550	3	-	0/4/4/4	0/1/1/1
4	CHB	Q	550	3	-	0/4/4/4	0/1/1/1
4	CHB	Q	551	-	-	0/4/4/4	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	550	CHB	O2-C7	-2.90	1.21	1.30
4	R	551	CHB	C1-C7	2.68	1.55	1.49
4	R	550	CHB	C1-C7	2.65	1.55	1.49
4	Q	551	CHB	C1-C7	2.61	1.55	1.49
4	O	550	CHB	O2-C7	-2.57	1.22	1.30
4	Q	550	CHB	C1-C7	2.55	1.54	1.49
4	P	551	CHB	C1-C7	2.52	1.54	1.49
4	P	550	CHB	C1-C7	2.47	1.54	1.49
4	N	550	CHB	C1-C7	2.31	1.54	1.49
4	N	551	CHB	C1-C7	2.30	1.54	1.49
4	Q	551	CHB	O2-C7	-2.23	1.23	1.30
4	O	551	CHB	O2-C7	-2.23	1.23	1.30
4	O	551	CHB	C1-C7	2.20	1.54	1.49
4	M	551	CHB	C1-C7	2.17	1.54	1.49
4	O	550	CHB	C1-C7	2.17	1.54	1.49
4	Q	550	CHB	O2-C7	-2.07	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	551	CHB	O2-C7	-2.06	1.24	1.30
4	P	551	CHB	O2-C7	-2.06	1.24	1.30
4	M	550	CHB	O2-C7	-2.02	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	551	CHB	O2-C7-O1	-3.20	116.47	123.35
4	N	551	CHB	O2-C7-C1	2.92	122.32	114.84
4	O	550	CHB	C5-C4-C3	2.77	121.09	118.49
4	Q	550	CHB	C5-C4-C3	2.62	120.96	118.49
4	P	551	CHB	O2-C7-C1	2.43	121.08	114.84
4	R	551	CHB	O2-C7-C1	2.33	120.81	114.84
4	O	551	CHB	O2-C7-C1	2.29	120.72	114.84
4	O	551	CHB	C5-C4-C3	2.28	120.64	118.49
4	N	550	CHB	C5-C4-C3	2.15	120.52	118.49
4	M	551	CHB	O2-C7-C1	2.04	120.08	114.84
4	Q	550	CHB	C2-C3-C4	-2.02	119.75	120.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	550	CHB	2	0
4	M	550	CHB	1	0
4	O	550	CHB	2	0
4	R	550	CHB	2	0
4	Q	550	CHB	2	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.