



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:33 PM UTC

PDB ID : 3PCF / pdb_00003pcf
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3-FLURO-4-HYDROXYBENZOATE
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-06-27
Resolution : 2.15 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

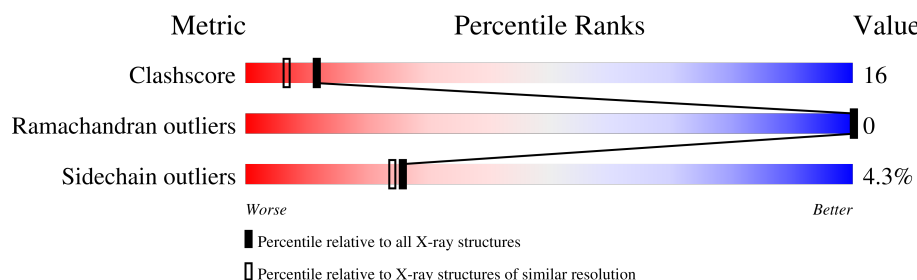
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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	68% 24% 6% .
1	B	200	64% 30% 6%
1	C	200	62% 30% 7% .
1	D	200	64% 30% 6%
1	E	200	54% 38% . .
1	F	200	57% 34% 8% .
2	M	238	61% 29% 8% . .
2	N	238	63% 29% 5% .

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Mol	Chain	Length	Quality of chain
2	O	238	 63% 29% 5% •
2	P	238	 61% 31% 6% •
2	Q	238	 59% 32% 7% •
2	R	238	 58% 32% 6% ••

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			

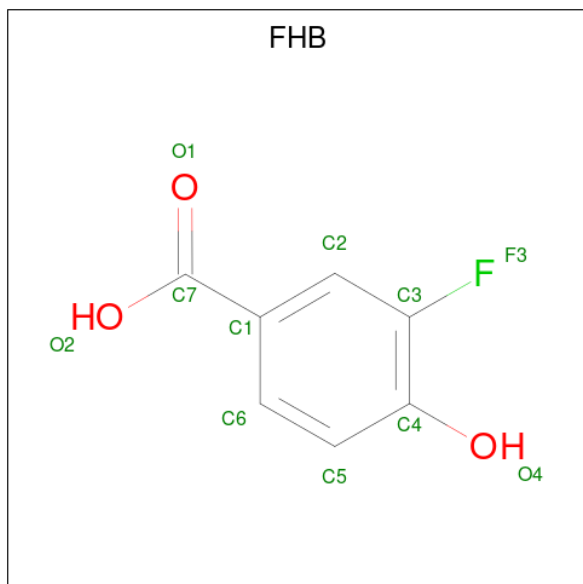
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

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-FLUORO-4-HYDROXYBENZOIC ACID (CCD ID: FHB) (formula: $C_7H_5FO_3$).



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

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

- Molecule 5 is water.

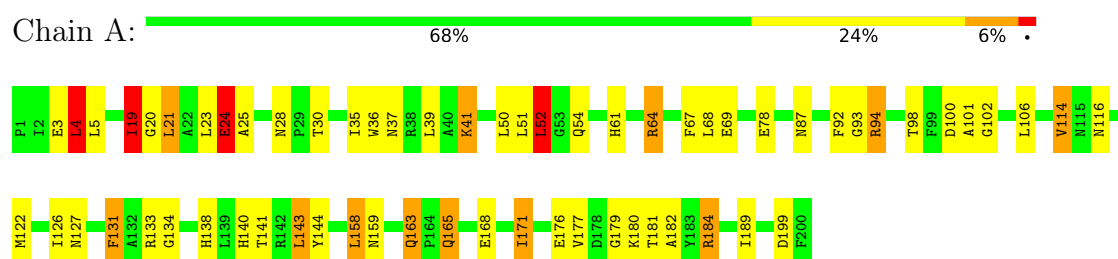
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		
5	M	158	Total	O	0	0
			158	158		
5	B	80	Total	O	0	0
			80	80		
5	N	166	Total	O	0	0
			166	166		
5	C	86	Total	O	0	0
			86	86		
5	O	155	Total	O	0	0
			155	155		
5	D	80	Total	O	0	0
			80	80		
5	P	155	Total	O	0	0
			155	155		
5	E	84	Total	O	0	0
			84	84		
5	Q	159	Total	O	0	0
			159	159		
5	F	83	Total	O	0	0
			83	83		
5	R	161	Total	O	0	0
			161	161		

3 Residue-property plots

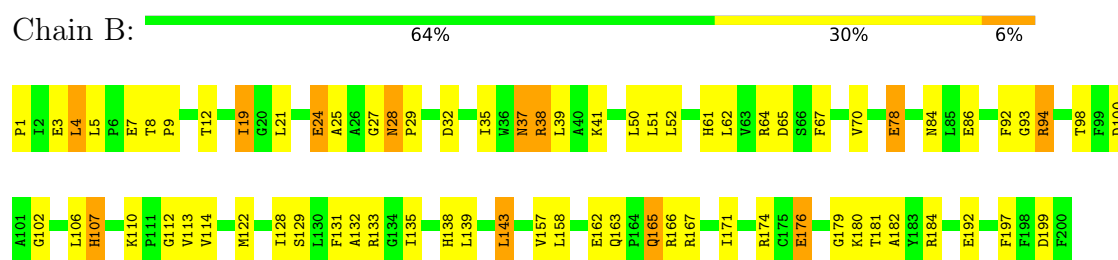
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

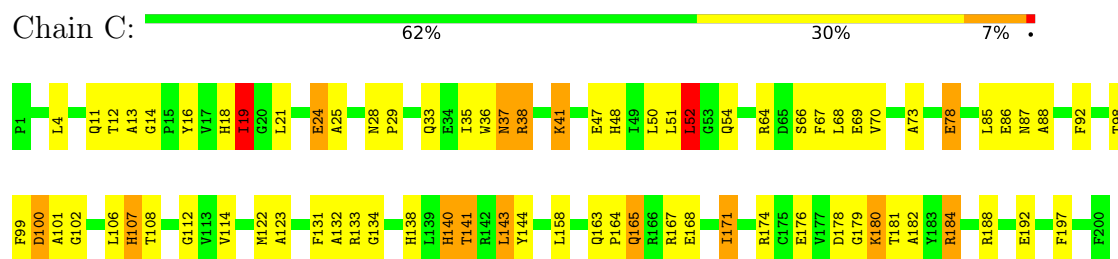
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



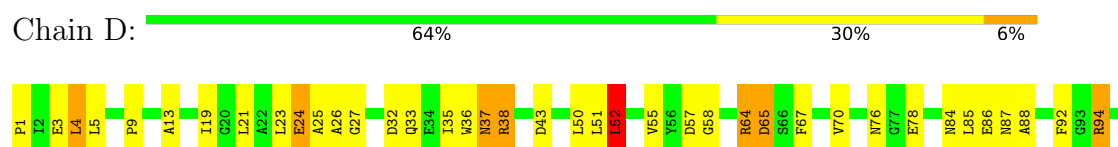
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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

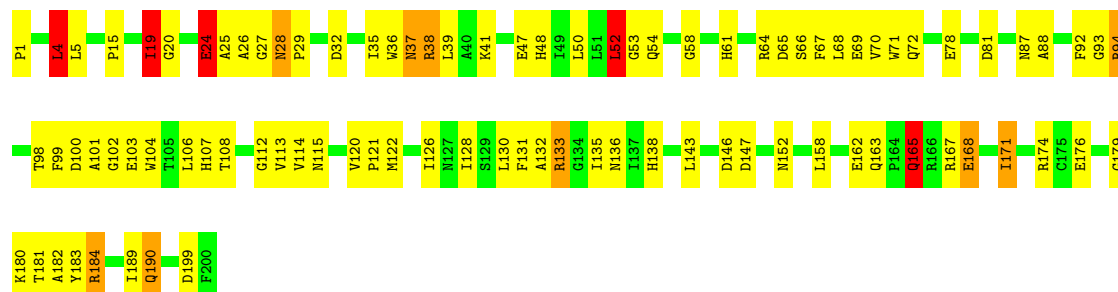


- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

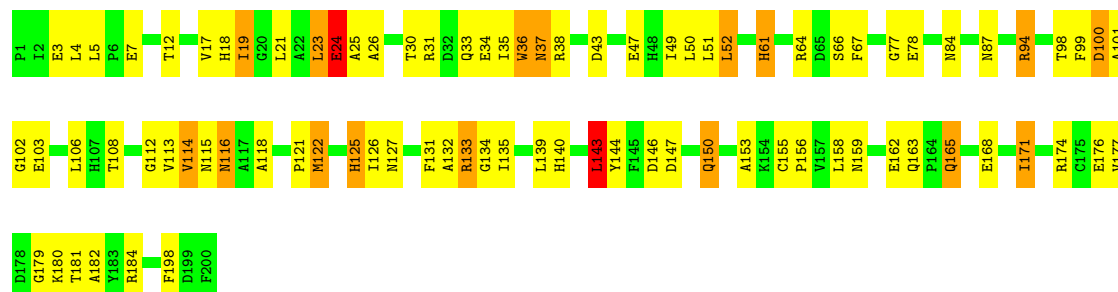




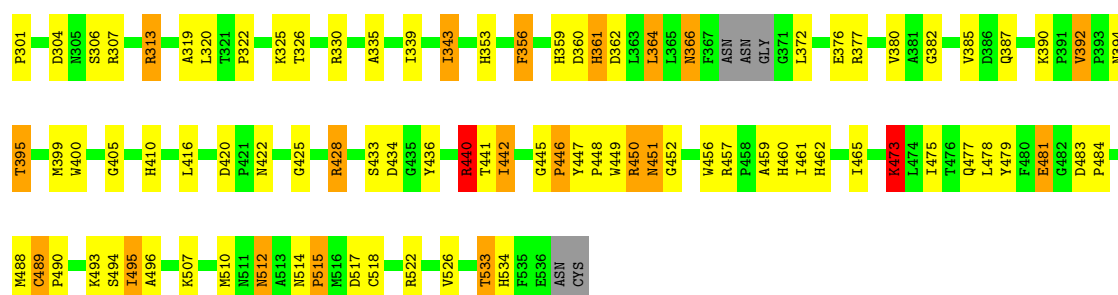
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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

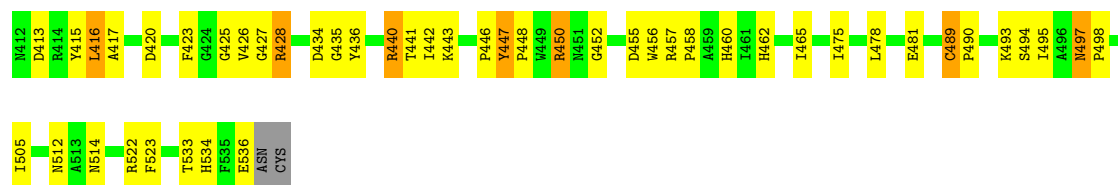


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



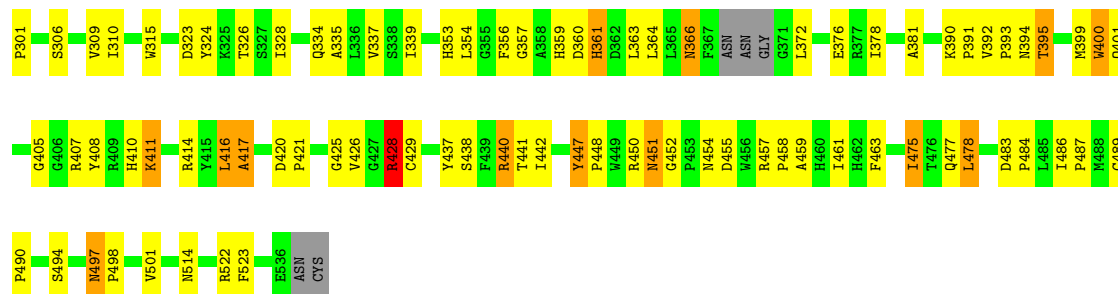
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain





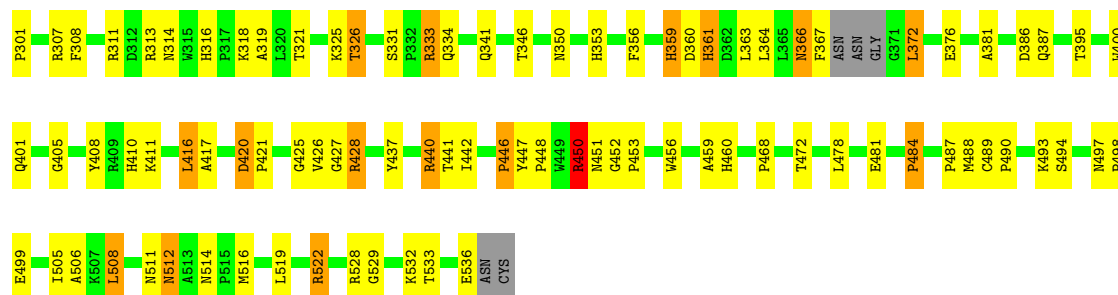
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O: 63% 29% 5% .



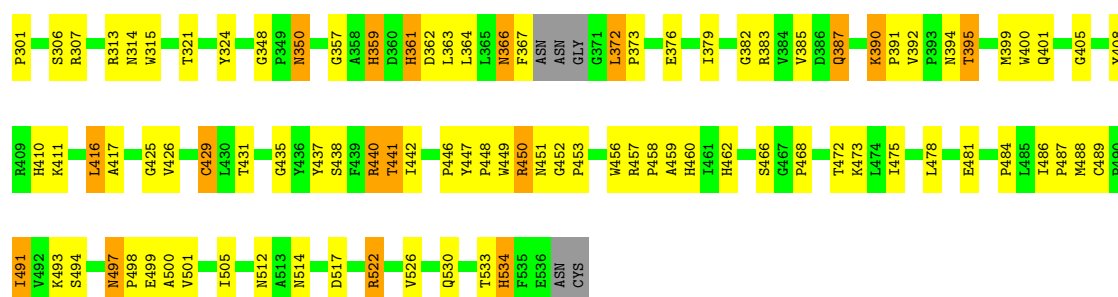
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain P: 61% 31% 6% .



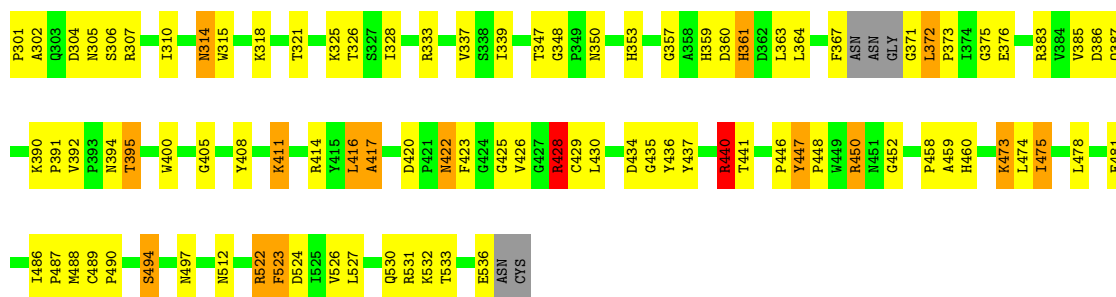
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain Q: 59% 32% 7% .



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

Chain R: 58% 32% 6% .



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	196.03Å 127.22Å 133.70Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	93.3 (6.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22080	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: FE, CME, FHB

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	1.29	2/1611 (0.1%)	1.93	36/2195 (1.6%)
1	B	1.29	4/1611 (0.2%)	1.82	26/2195 (1.2%)
1	C	1.32	3/1611 (0.2%)	1.81	29/2195 (1.3%)
1	D	1.33	2/1611 (0.1%)	1.88	32/2195 (1.5%)
1	E	1.37	2/1611 (0.1%)	1.84	30/2195 (1.4%)
1	F	1.37	4/1611 (0.2%)	1.86	38/2195 (1.7%)
2	M	1.48	9/1888 (0.5%)	2.00	53/2569 (2.1%)
2	N	1.40	4/1888 (0.2%)	1.90	32/2569 (1.2%)
2	O	1.45	7/1888 (0.4%)	1.93	41/2569 (1.6%)
2	P	1.47	8/1888 (0.4%)	1.95	54/2569 (2.1%)
2	Q	1.42	5/1888 (0.3%)	1.93	48/2569 (1.9%)
2	R	1.43	3/1888 (0.2%)	1.93	42/2569 (1.6%)
All	All	1.39	53/20994 (0.3%)	1.90	461/28584 (1.6%)

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	C	0	1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-9.96	1.32	1.46
2	P	451	ASN	CA-C	9.88	1.57	1.52
2	O	451	ASN	CA-C	9.46	1.56	1.52
2	M	451	ASN	CA-C	8.71	1.56	1.52
2	P	428	ARG	CD-NE	-8.07	1.34	1.46
1	E	108	THR	CA-CB	7.83	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	441	THR	CA-CB	7.06	1.62	1.54
2	P	321	THR	N-CA	7.03	1.54	1.46
2	R	375	GLY	N-CA	7.03	1.52	1.45
2	Q	451	ASN	CA-C	6.95	1.55	1.52
2	Q	392	VAL	N-CA	6.71	1.51	1.46
2	P	427	GLY	N-CA	6.66	1.51	1.45
2	N	495	ILE	CA-CB	6.49	1.61	1.53
2	O	441	THR	CA-CB	6.47	1.62	1.54
2	R	452	GLY	N-CA	6.35	1.53	1.44
1	F	108	THR	CA-CB	6.34	1.61	1.54
2	M	445	GLY	N-CA	6.31	1.53	1.44
2	Q	441	THR	CA-CB	6.26	1.63	1.53
2	M	495	ILE	CA-CB	6.21	1.60	1.53
2	M	440	ARG	CD-NE	-6.08	1.37	1.46
2	P	441	THR	CA-CB	6.07	1.62	1.53
1	F	94	ARG	CD-NE	-6.05	1.37	1.46
1	B	128	ILE	CA-CB	6.01	1.62	1.54
1	C	66	SER	CA-CB	-5.85	1.43	1.53
1	C	108	THR	CA-CB	5.81	1.61	1.53
2	P	508	LEU	N-CA	5.81	1.53	1.46
1	A	4	LEU	N-CA	5.75	1.52	1.45
2	P	506	ALA	N-CA	5.66	1.52	1.46
1	F	122	MET	N-CA	5.65	1.52	1.45
2	O	309	VAL	C-N	-5.65	1.27	1.33
2	P	528	ARG	NE-CZ	5.62	1.39	1.33
1	E	5	LEU	CA-C	5.61	1.59	1.53
1	B	5	LEU	CA-C	5.60	1.59	1.53
2	O	452	GLY	CA-C	5.60	1.59	1.51
2	O	401	GLN	N-CA	5.55	1.52	1.46
1	B	12	THR	CA-CB	5.50	1.62	1.53
1	B	94	ARG	CD-NE	-5.49	1.38	1.46
2	Q	449	TRP	N-CA	5.47	1.52	1.45
2	M	428	ARG	CD-NE	-5.45	1.38	1.46
2	R	333	ARG	CA-CB	-5.43	1.45	1.54
1	D	94	ARG	CD-NE	-5.43	1.38	1.46
2	N	441	THR	CA-CB	5.37	1.60	1.54
2	N	465	ILE	CA-CB	5.33	1.61	1.54
2	M	477	GLN	N-CA	5.29	1.52	1.46
2	Q	321	THR	CA-CB	5.20	1.59	1.53
2	M	460	HIS	N-CA	5.18	1.52	1.46
2	O	428	ARG	CD-NE	-5.16	1.39	1.46
2	N	457	ARG	NE-CZ	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	ARG	N-CA	5.06	1.52	1.46
1	D	65	ASP	N-CA	5.03	1.51	1.46
2	O	310	ILE	CA-CB	5.01	1.59	1.54
1	F	143	LEU	N-CA	5.01	1.52	1.46
2	M	380	VAL	N-CA	5.00	1.52	1.46

All (461) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	22.86	156.41	124.40
1	D	133	ARG	CD-NE-CZ	15.40	145.96	124.40
2	Q	450	ARG	CD-NE-CZ	13.79	143.71	124.40
2	P	428	ARG	CG-CD-NE	12.06	138.53	112.00
2	P	440	ARG	NE-CZ-NH2	-10.89	109.40	119.20
1	A	94	ARG	CG-CD-NE	10.75	135.64	112.00
2	P	450	ARG	CB-CG-CD	10.63	135.75	111.30
2	Q	499	GLU	CB-CG-CD	10.62	130.65	112.60
2	R	339	ILE	O-C-N	10.45	128.27	121.69
2	O	353	HIS	CA-CB-CG	-10.37	103.43	113.80
2	Q	451	ASN	O-C-N	10.27	128.43	120.83
1	F	38	ARG	CD-NE-CZ	10.18	138.65	124.40
1	F	94	ARG	CD-NE-CZ	10.13	138.59	124.40
2	Q	452	GLY	N-CA-C	-10.02	100.11	112.23
2	P	361	HIS	CA-CB-CG	-9.97	103.83	113.80
2	M	428	ARG	CD-NE-CZ	9.92	138.29	124.40
2	O	451	ASN	O-C-N	9.92	128.17	120.83
2	P	428	ARG	CD-NE-CZ	9.87	138.21	124.40
2	P	452	GLY	N-CA-C	-9.73	100.45	112.23
1	E	24	GLU	CB-CG-CD	9.57	128.87	112.60
2	O	428	ARG	CD-NE-CZ	9.56	137.79	124.40
2	R	361	HIS	CA-CB-CG	-9.36	104.44	113.80
2	M	452	GLY	N-CA-C	-9.02	101.32	112.23
2	M	494	SER	N-CA-C	-8.84	101.54	111.71
2	M	440	ARG	NE-CZ-NH2	-8.83	111.25	119.20
2	Q	361	HIS	CA-CB-CG	-8.79	105.01	113.80
1	C	133	ARG	CD-NE-CZ	8.73	136.62	124.40
2	O	394	ASN	CA-CB-CG	-8.51	104.09	112.60
2	M	428	ARG	NE-CZ-NH1	8.49	129.99	121.50
2	O	452	GLY	N-CA-C	-8.31	101.88	112.10
1	A	94	ARG	CB-CG-CD	8.23	130.22	111.30
2	P	536	GLU	CA-C-O	8.23	134.79	120.80
1	B	94	ARG	CB-CG-CD	8.22	130.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	HIS	CA-CB-CG	-8.16	105.64	113.80
2	Q	348	GLY	O-C-N	8.12	129.89	121.77
1	C	66	SER	CA-CB-OG	8.08	127.25	111.10
1	D	94	ARG	NE-CZ-NH2	-8.07	111.93	119.20
2	M	512	ASN	CA-CB-CG	-8.05	104.55	112.60
2	R	522	ARG	CD-NE-CZ	7.99	135.59	124.40
1	A	23	LEU	CB-CA-C	7.99	123.59	110.81
2	P	512	ASN	CA-CB-CG	-7.91	104.69	112.60
2	R	394	ASN	CA-CB-CG	-7.88	104.72	112.60
2	O	494	SER	N-CA-C	-7.67	103.18	112.54
1	F	43	ASP	CA-CB-CG	-7.66	104.94	112.60
2	Q	440	ARG	NE-CZ-NH2	-7.63	112.33	119.20
2	P	522	ARG	CD-NE-CZ	7.61	135.06	124.40
2	R	353	HIS	CA-CB-CG	-7.56	106.24	113.80
2	R	494	SER	N-CA-C	-7.55	103.53	112.89
1	A	24	GLU	CB-CG-CD	7.51	125.37	112.60
2	M	306	SER	N-CA-C	7.48	121.73	110.14
2	N	353	HIS	CA-CB-CG	-7.45	106.35	113.80
2	M	462	HIS	CA-CB-CG	-7.44	106.36	113.80
2	R	481	GLU	CB-CG-CD	7.43	125.24	112.60
2	O	463	PHE	CA-CB-CG	7.38	121.18	113.80
2	M	319	ALA	CA-C-O	-7.37	113.11	120.70
2	P	316	HIS	CA-CB-CG	-7.34	106.46	113.80
1	D	37	ASN	N-CA-C	7.33	121.14	112.93
2	O	514	ASN	CA-CB-CG	7.32	119.92	112.60
2	R	447	TYR	O-C-N	7.30	127.53	121.83
1	B	37	ASN	N-CA-C	7.29	121.09	112.93
2	N	333	ARG	N-CA-C	-7.27	104.93	114.31
1	F	23	LEU	CB-CA-C	7.27	122.48	110.92
2	P	451	ASN	O-C-N	7.25	126.19	120.83
2	O	497	ASN	CB-CA-C	7.20	118.36	110.08
2	M	481	GLU	CB-CG-CD	7.19	124.82	112.60
1	D	94	ARG	CB-CG-CD	7.17	127.78	111.30
2	Q	387	GLN	OE1-CD-NE2	7.16	129.76	122.60
2	M	428	ARG	CG-CD-NE	7.12	127.66	112.00
2	P	326	THR	CA-CB-OG1	-7.12	98.92	109.60
2	N	452	GLY	N-CA-C	-7.10	97.86	112.34
1	B	94	ARG	CG-CD-NE	7.09	127.60	112.00
1	F	133	ARG	CD-NE-CZ	7.06	134.28	124.40
1	A	5	LEU	N-CA-C	-7.05	100.87	109.83
2	M	514	ASN	O-C-N	7.05	127.82	121.19
2	R	314	ASN	N-CA-C	-7.04	104.56	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	ARG	NE-CZ-NH1	7.04	128.54	121.50
1	B	184	ARG	NE-CZ-NH2	-7.04	112.86	119.20
2	O	366	ASN	N-CA-C	7.04	121.70	113.18
2	N	440	ARG	NE-CZ-NH2	-7.00	112.90	119.20
2	M	353	HIS	CA-CB-CG	-6.99	106.81	113.80
2	M	361	HIS	CA-CB-CG	-6.98	106.82	113.80
2	N	512	ASN	CA-CB-CG	-6.94	105.66	112.60
1	D	188	ARG	CD-NE-CZ	-6.93	114.69	124.40
2	M	440	ARG	NE-CZ-NH1	6.93	128.43	121.50
2	R	497	ASN	CB-CA-C	6.93	117.75	109.85
1	E	99	PHE	CA-CB-CG	6.90	120.70	113.80
1	F	125	HIS	CA-CB-CG	-6.89	106.91	113.80
1	D	64	ARG	CD-NE-CZ	-6.89	114.76	124.40
2	Q	359	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	159	ASN	CA-CB-CG	-6.88	105.72	112.60
2	N	361	HIS	CA-CB-CG	-6.87	106.93	113.80
1	E	38	ARG	NE-CZ-NH2	-6.86	113.03	119.20
2	O	447	TYR	O-C-N	6.86	126.65	121.85
2	N	372	LEU	N-CA-CB	-6.84	101.05	110.29
1	A	36	TRP	CB-CA-C	6.84	124.03	110.42
2	P	428	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	F	36	TRP	CB-CA-C	6.80	123.94	110.42
2	Q	452	GLY	CA-C-O	-6.77	115.41	122.38
2	R	434	ASP	CA-CB-CG	-6.75	105.85	112.60
2	R	440	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	A	177	VAL	O-C-N	6.74	129.04	122.97
2	P	314	ASN	N-CA-C	-6.73	105.11	113.38
2	O	392	VAL	O-C-N	6.71	127.40	120.96
2	P	353	HIS	CA-CB-CG	-6.70	107.10	113.80
1	C	37	ASN	N-CA-C	6.69	121.12	113.15
2	P	450	ARG	CG-CD-NE	6.68	126.69	112.00
1	A	37	ASN	CA-CB-CG	-6.67	105.93	112.60
1	F	158	LEU	CB-CA-C	6.67	122.96	110.63
2	R	450	ARG	CD-NE-CZ	6.67	133.73	124.40
2	M	451	ASN	O-C-N	6.63	125.74	120.83
2	O	309	VAL	CA-C-N	6.62	129.63	120.49
2	O	309	VAL	C-N-CA	6.62	129.63	120.49
2	O	411	LYS	CB-CA-C	-6.62	99.76	110.74
1	C	87	ASN	CA-CB-CG	6.61	119.21	112.60
1	C	66	SER	N-CA-CB	6.59	119.66	110.17
1	F	5	LEU	N-CA-C	-6.57	101.49	109.83
2	M	319	ALA	O-C-N	6.56	129.17	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	512	ASN	CA-CB-CG	-6.56	106.04	112.60
2	Q	534	HIS	CA-CB-CG	6.55	120.36	113.80
2	M	382	GLY	CA-C-O	6.52	128.20	121.35
2	P	428	ARG	CB-CG-CD	6.51	126.28	111.30
1	A	163	GLN	CA-C-O	6.51	123.52	119.29
2	M	450	ARG	CA-C-N	6.47	130.52	121.79
2	M	450	ARG	C-N-CA	6.47	130.52	121.79
2	Q	314	ASN	OD1-CG-ND2	6.47	129.07	122.60
2	O	451	ASN	CA-CB-CG	-6.47	106.13	112.60
2	P	314	ASN	CB-CA-C	6.45	120.86	109.65
2	Q	350	ASN	CA-CB-CG	-6.43	106.17	112.60
1	F	94	ARG	CG-CD-NE	6.43	126.15	112.00
1	C	38	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	C	19	ILE	CA-CB-CG2	6.41	121.39	110.50
2	R	411	LYS	CB-CA-C	-6.41	100.10	110.74
1	F	94	ARG	CB-CG-CD	6.40	126.01	111.30
1	B	5	LEU	N-CA-C	-6.39	101.71	109.83
1	D	5	LEU	N-CA-C	-6.39	101.72	109.83
2	O	395	THR	CA-CB-OG1	-6.36	100.06	109.60
1	E	113	VAL	N-CA-CB	-6.34	103.81	110.72
1	F	37	ASN	N-CA-C	6.33	120.02	112.93
2	R	428	ARG	NE-CZ-NH2	-6.32	113.51	119.20
2	M	440	ARG	CD-NE-CZ	6.32	133.25	124.40
1	D	171	ILE	N-CA-CB	-6.32	103.80	111.00
1	C	47	GLU	CB-CG-CD	6.32	123.34	112.60
1	F	5	LEU	O-C-N	6.30	128.49	121.43
2	Q	457	ARG	NE-CZ-NH1	6.28	127.78	121.50
1	A	52	LEU	CB-CA-C	6.28	123.94	110.45
2	N	497	ASN	CB-CA-C	6.27	118.41	109.38
1	D	162	GLU	CA-CB-CG	6.26	126.63	114.10
1	F	24	GLU	CB-CG-CD	6.26	123.24	112.60
2	P	372	LEU	CB-CA-C	6.25	117.37	108.68
2	Q	494	SER	N-CA-C	-6.24	104.93	112.54
1	D	38	ARG	CD-NE-CZ	-6.23	115.67	124.40
1	D	52	LEU	CB-CA-C	6.23	123.21	109.94
2	Q	357	GLY	N-CA-C	-6.23	104.22	112.82
1	E	5	LEU	N-CA-C	-6.21	101.50	110.08
2	Q	379	ILE	O-C-N	6.21	129.70	123.18
2	P	508	LEU	O-C-N	6.21	130.50	122.87
1	E	189	ILE	O-C-N	6.20	127.89	121.87
2	R	387	GLN	OE1-CD-NE2	6.18	128.78	122.60
1	A	116	ASN	CA-CB-CG	6.18	118.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	458	PRO	N-CA-C	-6.17	102.15	111.41
1	A	64	ARG	CD-NE-CZ	-6.17	115.77	124.40
1	A	133	ARG	NE-CZ-NH2	-6.15	113.66	119.20
2	M	512	ASN	OD1-CG-ND2	6.14	128.74	122.60
1	E	167	ARG	CD-NE-CZ	-6.14	115.81	124.40
2	R	359	HIS	CA-CB-CG	-6.13	107.67	113.80
1	D	171	ILE	CB-CA-C	6.13	118.38	110.96
1	E	47	GLU	CB-CG-CD	6.13	123.02	112.60
2	R	357	GLY	N-CA-C	-6.12	104.70	112.54
2	M	489	CYS	O-C-N	6.12	126.51	121.31
2	M	496	ALA	N-CA-C	6.12	118.92	111.82
1	E	37	ASN	N-CA-C	6.12	120.24	113.21
1	A	30	THR	CA-CB-OG1	-6.11	100.43	109.60
1	C	41	LYS	N-CA-C	-6.10	101.33	110.24
1	C	158	LEU	CB-CA-C	6.10	121.92	110.63
1	A	37	ASN	N-CA-C	6.10	119.67	112.72
2	O	361	HIS	CA-CB-CG	-6.10	107.70	113.80
2	R	333	ARG	N-CA-CB	6.09	119.60	110.65
1	B	94	ARG	CD-NE-CZ	6.08	132.92	124.40
2	Q	394	ASN	CA-CB-CG	-6.08	106.52	112.60
2	R	523	PHE	CA-CB-CG	6.07	119.87	113.80
2	P	372	LEU	CA-C-O	6.07	125.83	120.19
1	B	192	GLU	CA-CB-CG	6.06	126.23	114.10
2	M	422	ASN	CA-CB-CG	-6.05	106.55	112.60
2	R	452	GLY	N-CA-C	-6.04	100.02	112.34
1	C	52	LEU	CB-CA-C	6.04	121.85	110.62
2	Q	522	ARG	NE-CZ-NH1	-6.04	115.46	121.50
2	N	514	ASN	O-C-N	6.04	126.95	120.85
1	C	134	GLY	N-CA-C	-6.03	107.37	115.21
2	M	479	TYR	CA-C-O	-6.02	114.28	121.56
1	A	141	THR	CA-CB-CG2	6.00	120.70	110.50
2	M	459	ALA	N-CA-C	-5.99	101.54	110.23
2	R	428	ARG	CD-NE-CZ	5.97	132.76	124.40
2	O	334	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	F	66	SER	CA-CB-OG	5.93	122.96	111.10
2	R	337	VAL	CA-C-O	-5.92	114.14	120.59
1	D	76	ASN	CA-CB-CG	-5.91	106.69	112.60
1	E	19	ILE	CB-CA-C	5.91	120.68	112.05
2	P	367	PHE	CA-C-O	-5.90	110.77	120.80
1	F	198	PHE	O-C-N	5.90	130.71	123.10
1	E	88	ALA	N-CA-C	-5.89	104.80	112.23
1	E	94	ARG	CG-CD-NE	5.88	124.94	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	LEU	CA-C-O	-5.88	112.54	119.48
2	M	320	LEU	CA-C-N	-5.88	116.51	122.74
2	M	320	LEU	C-N-CA	-5.88	116.51	122.74
2	P	459	ALA	N-CA-C	-5.87	101.35	110.10
2	O	417	ALA	N-CA-C	-5.87	102.65	109.93
1	E	136	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	3	GLU	CB-CG-CD	5.87	122.57	112.60
1	A	189	ILE	O-C-N	5.86	128.43	121.80
1	A	133	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	E	152	ASN	O-C-N	5.85	128.32	122.12
2	R	428	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	F	140	HIS	CA-C-O	5.84	126.79	120.43
1	C	21	LEU	N-CA-CB	-5.83	102.83	110.88
1	D	162	GLU	N-CA-CB	5.83	118.62	109.94
1	B	197	PHE	CA-CB-CG	5.83	119.63	113.80
2	M	473	LYS	CA-CB-CG	5.82	125.74	114.10
2	Q	366	ASN	N-CA-C	5.82	120.24	113.20
1	A	131	PHE	CA-CB-CG	5.81	119.61	113.80
1	B	129	SER	N-CA-CB	5.81	120.44	110.68
1	E	162	GLU	N-CA-C	5.80	118.10	111.02
2	M	313	ARG	CB-CA-C	5.80	121.14	110.11
2	O	457	ARG	CA-CB-CG	5.80	125.69	114.10
1	C	78	GLU	CB-CG-CD	5.79	122.44	112.60
1	C	69	GLU	CB-CG-CD	5.78	122.42	112.60
1	C	48	HIS	CA-CB-CG	-5.78	108.02	113.80
2	R	422	ASN	CA-CB-CG	-5.78	106.82	112.60
1	A	21	LEU	N-CA-C	5.77	121.04	113.30
2	O	337	VAL	CA-C-O	-5.77	114.30	120.59
2	M	473	LYS	N-CA-CB	5.77	118.17	109.34
1	D	171	ILE	N-CA-C	5.77	117.06	108.23
2	P	417	ALA	CB-CA-C	5.77	118.63	109.52
2	N	481	GLU	CA-CB-CG	5.77	125.63	114.10
2	M	460	HIS	O-C-N	5.76	129.58	123.42
2	Q	466	SER	N-CA-C	5.76	117.42	111.03
2	N	367	PHE	CA-C-O	-5.75	111.02	120.80
2	N	348	GLY	O-C-N	5.75	127.52	121.77
2	Q	497	ASN	N-CA-CB	-5.75	102.70	110.23
2	N	443	LYS	O-C-N	5.74	126.52	121.18
1	E	171	ILE	N-CA-CB	-5.73	104.51	111.21
1	B	107	HIS	CA-CB-CG	-5.72	108.08	113.80
1	D	87	ASN	OD1-CG-ND2	5.72	128.32	122.60
2	M	428	ARG	NE-CZ-NH2	-5.71	114.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	133	ARG	CD-NE-CZ	-5.71	116.41	124.40
2	Q	489	CYS	CA-C-O	5.71	123.54	119.32
1	A	140	HIS	CB-CA-C	-5.70	99.91	109.48
1	B	21	LEU	N-CA-CB	-5.70	102.01	110.61
2	R	417	ALA	N-CA-C	-5.69	102.61	109.83
1	C	180	LYS	N-CA-CB	5.68	119.83	110.69
1	B	9	PRO	CB-CA-C	-5.67	104.14	111.46
1	E	158	LEU	CB-CA-C	5.67	120.20	110.79
1	C	171	ILE	N-CA-C	5.67	116.26	107.99
1	B	110	LYS	CA-C-O	5.67	125.10	119.49
1	C	158	LEU	N-CA-CB	-5.66	101.50	110.22
2	P	514	ASN	CA-CB-CG	5.65	118.25	112.60
1	F	171	ILE	N-CA-C	5.65	116.87	108.23
2	O	354	LEU	N-CA-C	-5.65	101.92	110.28
2	N	417	ALA	CB-CA-C	5.64	118.27	109.42
2	P	333	ARG	CD-NE-CZ	5.63	132.28	124.40
1	D	166	ARG	CA-C-N	5.63	127.82	120.28
1	D	166	ARG	C-N-CA	5.63	127.82	120.28
2	O	454	ASN	CA-CB-CG	5.62	118.22	112.60
2	P	319	ALA	O-C-N	5.62	128.16	122.09
2	O	501	VAL	N-CA-CB	5.62	117.13	110.55
2	R	475	ILE	N-CA-CB	5.61	121.16	111.39
2	Q	324	TYR	N-CA-C	-5.61	97.43	107.98
2	N	446	PRO	CB-CA-C	-5.60	103.61	110.95
1	F	177	VAL	CB-CA-C	5.60	117.39	110.73
1	B	171	ILE	N-CA-C	5.59	116.15	107.99
2	O	458	PRO	N-CA-C	-5.58	103.03	111.41
2	M	339	ILE	O-C-N	5.58	127.46	121.10
2	M	457	ARG	N-CA-C	-5.58	103.01	109.93
2	O	378	ILE	O-C-N	5.58	129.36	123.00
2	P	311	ARG	CG-CD-NE	-5.58	99.72	112.00
2	P	386	ASP	CB-CA-C	5.58	120.10	110.45
2	Q	401	GLN	O-C-N	5.58	128.96	122.99
2	N	494	SER	N-CA-C	-5.57	105.31	111.71
1	F	61	HIS	CA-CB-CG	-5.57	108.23	113.80
1	D	133	ARG	N-CA-C	-5.57	102.04	110.28
2	P	325	LYS	N-CA-C	5.56	117.78	111.11
2	P	316	HIS	O-C-N	5.55	127.49	121.60
2	Q	497	ASN	CA-C-N	5.55	125.38	119.28
2	Q	497	ASN	C-N-CA	5.55	125.38	119.28
2	Q	497	ASN	CB-CA-C	5.54	117.36	109.38
2	Q	411	LYS	CB-CA-C	-5.54	101.65	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	ASP	N-CA-C	5.52	118.22	111.82
2	M	507	LYS	CA-CB-CG	5.51	125.13	114.10
2	R	459	ALA	N-CA-C	-5.51	102.24	110.23
1	D	57	ASP	CA-CB-CG	5.51	118.11	112.60
2	M	420	ASP	CB-CA-C	5.50	116.48	110.15
2	M	446	PRO	N-CA-C	-5.50	103.52	111.22
1	F	162	GLU	N-CA-CB	5.50	118.18	109.82
2	N	420	ASP	O-C-N	5.50	128.11	121.29
2	Q	491	ILE	N-CA-CB	5.50	118.01	110.54
1	E	4	LEU	CA-C-O	-5.49	114.74	121.88
1	F	127	ASN	CA-CB-CG	-5.48	107.12	112.60
2	O	315	TRP	CA-C-O	5.48	126.41	120.55
2	R	512	ASN	CA-CB-CG	-5.47	107.13	112.60
1	C	14	GLY	CA-C-N	5.46	125.07	119.56
1	C	14	GLY	C-N-CA	5.46	125.07	119.56
1	D	94	ARG	CG-CD-NE	5.46	124.00	112.00
2	Q	459	ALA	N-CA-C	-5.46	101.97	110.10
2	R	420	ASP	CB-CA-C	5.45	116.22	110.17
2	M	394	ASN	CA-CB-CG	-5.44	107.16	112.60
2	Q	382	GLY	O-C-N	5.44	129.14	123.92
1	D	55	VAL	CB-CA-C	5.44	118.68	110.63
1	E	107	HIS	CA-CB-CG	-5.43	108.36	113.80
1	E	165	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	158	LEU	CB-CA-C	5.42	119.90	110.68
2	P	334	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	O	461	ILE	O-C-N	5.41	128.93	123.20
1	B	139	LEU	O-C-N	5.40	129.66	123.29
2	Q	452	GLY	O-C-N	5.40	127.58	122.18
1	A	5	LEU	O-C-N	5.39	127.47	121.43
2	P	410	HIS	CA-C-N	5.39	128.91	120.82
2	P	410	HIS	C-N-CA	5.39	128.91	120.82
1	F	150	GLN	O-C-N	5.39	127.64	122.03
2	R	315	TRP	N-CA-C	-5.39	104.83	111.40
2	M	392	VAL	O-C-N	5.38	127.23	121.10
2	N	440	ARG	CD-NE-CZ	-5.38	116.87	124.40
2	Q	512	ASN	OD1-CG-ND2	5.37	127.97	122.60
2	R	423	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	112	GLY	N-CA-C	-5.37	104.20	112.85
1	D	9	PRO	CB-CA-C	-5.37	104.53	111.46
1	F	94	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	F	114	VAL	CA-C-O	-5.37	116.03	121.67
1	A	134	GLY	N-CA-C	-5.36	108.31	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	NE-CZ-NH1	5.36	126.86	121.50
2	P	481	GLU	CA-CB-CG	5.36	124.83	114.10
2	R	367	PHE	CA-C-O	-5.36	111.68	120.80
2	R	446	PRO	N-CA-C	-5.35	103.73	111.22
2	Q	314	ASN	N-CA-C	-5.35	106.80	113.38
1	C	107	HIS	CA-CB-CG	-5.35	108.45	113.80
2	M	462	HIS	O-C-N	5.34	129.31	123.22
2	N	447	TYR	CA-C-O	5.34	124.47	119.13
2	P	532	LYS	O-C-N	5.34	129.00	122.96
2	M	356	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	94	ARG	NE-CZ-NH2	-5.33	114.40	119.20
2	N	395	THR	CA-CB-OG1	-5.33	101.60	109.60
1	C	178	ASP	CA-CB-CG	-5.33	107.27	112.60
1	A	184	ARG	O-C-N	5.33	129.58	123.29
2	O	411	LYS	O-C-N	5.33	128.24	122.11
2	N	411	LYS	CB-CA-C	-5.33	102.00	110.84
1	B	162	GLU	CA-CB-CG	5.32	124.73	114.10
2	P	359	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	163	GLN	CB-CA-C	5.31	116.19	110.08
2	P	441	THR	O-C-N	5.31	129.58	122.73
1	D	13	ALA	O-C-N	5.31	129.44	122.33
1	D	23	LEU	CB-CA-C	5.30	120.97	110.42
2	O	339	ILE	O-C-N	5.30	125.03	121.69
2	N	455	ASP	CA-CB-CG	-5.29	107.31	112.60
2	P	533	THR	CA-CB-OG1	-5.29	101.66	109.60
1	E	120	VAL	N-CA-CB	-5.29	104.73	111.23
1	D	88	ALA	N-CA-C	-5.28	105.57	112.23
2	R	376	GLU	CG-CD-OE2	-5.28	106.26	118.40
2	P	372	LEU	N-CA-CB	-5.28	101.41	110.11
2	N	489	CYS	CB-CA-C	5.26	117.93	109.51
2	Q	446	PRO	N-CA-C	-5.26	103.52	111.41
2	R	325	LYS	N-CA-C	5.25	120.04	111.37
2	M	325	LYS	CA-C-O	-5.25	115.04	120.92
2	M	322	PRO	N-CA-C	5.25	123.28	112.47
2	M	366	ASN	N-CA-C	5.24	119.39	113.15
1	E	112	GLY	N-CA-C	-5.23	104.42	112.85
2	M	481	GLU	CA-C-N	5.23	130.93	122.09
2	M	481	GLU	C-N-CA	5.23	130.93	122.09
2	N	357	GLY	N-CA-C	-5.23	105.60	112.82
2	Q	417	ALA	N-CA-C	-5.23	103.19	109.83
1	E	48	HIS	CA-CB-CG	-5.23	108.57	113.80
1	E	24	GLU	CA-CB-CG	5.22	124.55	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ARG	N-CA-CB	-5.21	100.86	110.56
2	M	518	CYS	CA-C-O	5.21	126.83	120.99
2	N	316	HIS	N-CA-C	-5.21	102.89	110.08
1	F	126	ILE	O-C-N	5.21	128.72	123.20
2	R	348	GLY	O-C-N	5.21	126.98	121.77
1	A	41	LYS	N-CA-C	-5.21	103.11	110.29
2	N	465	ILE	O-C-N	5.21	128.82	123.20
2	Q	324	TYR	O-C-N	5.21	129.20	122.43
1	A	19	ILE	CB-CA-C	5.20	120.22	112.16
2	N	489	CYS	N-CA-C	5.20	117.12	109.42
2	N	458	PRO	N-CA-C	-5.20	103.28	111.34
2	Q	367	PHE	CA-C-O	-5.20	111.96	120.80
1	F	116	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	B	41	LYS	N-CA-C	-5.19	103.12	110.29
2	Q	450	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
2	P	484	PRO	CB-CA-C	5.19	119.26	111.68
1	E	71	TRP	CB-CA-C	5.19	118.62	109.80
2	P	333	ARG	CB-CA-C	5.19	117.78	109.07
1	A	171	ILE	N-CA-C	5.18	115.56	107.99
1	C	112	GLY	N-CA-C	-5.18	104.51	112.85
2	O	400	TRP	N-CA-CB	5.18	120.46	111.39
1	F	7	GLU	CB-CG-CD	5.18	121.40	112.60
1	C	141	THR	CA-CB-CG2	5.17	119.29	110.50
1	E	28	ASN	O-C-N	5.17	125.74	121.35
2	O	428	ARG	NE-CZ-NH1	5.16	126.66	121.50
2	Q	395	THR	CA-CB-OG1	-5.16	101.85	109.60
1	D	21	LEU	N-CA-C	5.16	120.21	112.94
1	B	113	VAL	N-CA-C	5.15	116.22	109.21
1	F	158	LEU	N-CA-CB	-5.15	102.28	110.22
1	B	8	THR	CA-C-O	5.15	124.59	119.75
1	F	106	LEU	N-CA-CB	-5.15	101.95	111.53
1	C	140	HIS	N-CA-CB	5.15	119.01	110.52
1	C	192	GLU	CB-CG-CD	5.14	121.35	112.60
1	F	30	THR	CA-CB-OG1	-5.14	101.88	109.60
2	O	440	ARG	NE-CZ-NH2	-5.14	114.58	119.20
2	P	331	SER	O-C-N	5.14	126.76	121.72
2	Q	458	PRO	N-CA-C	-5.14	103.38	111.34
2	R	328	ILE	N-CA-C	5.14	115.75	110.36
2	O	475	ILE	N-CA-CB	5.13	118.50	111.41
1	E	190	GLN	N-CA-CB	-5.13	101.97	111.52
1	A	127	ASN	OD1-CG-ND2	5.13	127.73	122.60
2	P	446	PRO	N-CA-C	-5.12	104.05	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	LEU	CB-CA-C	5.12	119.29	110.79
2	N	417	ALA	N-CA-C	-5.12	103.33	109.83
1	F	112	GLY	N-CA-C	-5.12	104.61	112.85
1	B	166	ARG	N-CA-CB	5.12	118.89	110.39
2	Q	451	ASN	N-CA-C	-5.11	100.32	108.30
2	M	339	ILE	N-CA-CB	5.11	118.36	111.21
2	Q	501	VAL	O-C-N	5.11	126.83	121.87
2	P	420	ASP	CB-CA-C	5.11	116.02	110.15
2	P	512	ASN	OD1-CG-ND2	5.10	127.70	122.60
2	Q	514	ASN	O-C-N	5.10	126.00	120.85
1	D	140	HIS	CB-CA-C	-5.10	101.33	109.75
2	O	323	ASP	CA-CB-CG	-5.10	107.50	112.60
1	B	28	ASN	O-C-N	5.09	125.68	121.35
2	P	505	ILE	N-CA-C	5.07	115.06	107.51
1	F	139	LEU	CA-C-N	5.07	129.71	122.72
1	F	139	LEU	C-N-CA	5.07	129.71	122.72
1	B	157	VAL	CB-CA-C	5.06	118.67	112.04
2	P	350	ASN	CA-CB-CG	-5.06	107.54	112.60
2	M	515	PRO	CB-CA-C	5.06	117.99	111.56
2	N	458	PRO	CB-CA-C	-5.06	104.59	111.12
1	C	13	ALA	N-CA-C	-5.06	105.95	111.82
2	Q	499	GLU	CG-CD-OE1	5.06	130.04	118.40
2	P	401	GLN	O-C-N	5.06	128.40	122.99
2	R	339	ILE	N-CA-C	-5.06	105.04	109.19
1	A	61	HIS	CA-C-N	5.06	127.95	120.82
1	A	61	HIS	C-N-CA	5.06	127.95	120.82
1	B	167	ARG	CD-NE-CZ	5.06	131.48	124.40
2	P	366	ASN	N-CA-C	5.06	119.08	113.01
2	N	450	ARG	CB-CG-CD	5.05	122.91	111.30
2	O	357	GLY	N-CA-C	-5.05	106.08	112.54
2	O	459	ALA	N-CA-C	-5.05	102.58	110.10
2	P	494	SER	N-CA-C	-5.04	106.22	112.38
2	P	508	LEU	CA-C-O	-5.04	115.64	121.19
2	M	533	THR	CA-CB-OG1	-5.04	102.04	109.60
2	R	441	THR	O-C-N	5.04	128.98	122.68
1	D	112	GLY	CA-C-N	5.04	129.26	121.71
1	D	112	GLY	C-N-CA	5.04	129.26	121.71
1	F	33	GLN	CB-CA-C	5.04	118.06	109.75
1	F	100	ASP	CA-CB-CG	-5.03	107.57	112.60
2	O	410	HIS	CA-C-N	5.03	128.36	120.82
2	O	410	HIS	C-N-CA	5.03	128.36	120.82
2	R	305	ASN	CB-CA-C	5.02	117.99	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	GLU	CA-CB-CG	5.02	124.14	114.10
1	E	52	LEU	CB-CA-C	5.02	121.24	110.45
1	F	171	ILE	CB-CA-C	-5.02	104.89	110.96
2	Q	481	GLU	CB-CG-CD	5.01	121.12	112.60
2	O	306	SER	N-CA-C	5.01	116.81	109.24
2	P	508	LEU	N-CA-C	-5.01	102.97	110.23
2	N	457	ARG	O-C-N	5.00	126.28	121.28
2	M	442	ILE	CB-CA-C	5.00	118.52	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	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	47	0
1	B	1571	0	1499	51	0
1	C	1571	0	1499	66	0
1	D	1571	0	1499	59	0
1	E	1571	0	1499	62	0
1	F	1571	0	1499	82	0
2	M	1844	0	1796	62	0
2	N	1844	0	1796	54	0
2	O	1844	0	1796	46	0
2	P	1844	0	1796	61	0
2	Q	1844	0	1796	67	0
2	R	1844	0	1796	71	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	22	0	7	0	0
4	N	22	0	7	0	0
4	O	22	0	7	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	85	0	0	3	0
5	B	80	0	0	2	0
5	C	86	0	0	1	0
5	D	80	0	0	1	0
5	E	84	0	0	3	0
5	F	83	0	0	2	0
5	M	158	0	0	5	0
5	N	166	0	0	4	0
5	O	155	0	0	4	0
5	P	155	0	0	3	0
5	Q	159	0	0	7	0
5	R	161	0	0	4	0
All	All	22080	0	19812	644	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 16.

All (644) 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:64:ARG:NH1	1:D:100:ASP:O	1.87	1.07
1:F:64:ARG:NH1	1:F:100:ASP:O	1.87	1.06
1:B:165:GLN:H	1:B:165:GLN:NE2	1.58	1.00
1:E:165:GLN:H	1:E:165:GLN:NE2	1.59	0.97
1:C:64:ARG:NH1	1:C:100:ASP:O	1.97	0.96
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.81	0.93
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.83	0.93
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.31	0.92
1:E:64:ARG:NH1	1:E:100:ASP:O	2.01	0.92
2:M:390:LYS:HD2	5:M:640:HOH:O	1.70	0.92
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.52	0.90
1:E:165:GLN:HE21	1:E:165:GLN:N	1.69	0.90
1:D:165:GLN:H	1:D:165:GLN:HE21	1.17	0.90
1:F:168:GLU:HA	1:F:171:ILE:HD13	1.53	0.87
2:R:361:HIS:H	2:R:361:HIS:CD2	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:NE2	1:F:165:GLN:H	1.74	0.85
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.91	0.84
1:B:64:ARG:NH1	1:B:100:ASP:O	2.09	0.84
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.60	0.84
1:E:165:GLN:H	1:E:165:GLN:HE21	0.86	0.84
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.41	0.83
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.61	0.83
2:R:361:HIS:H	2:R:361:HIS:HD2	1.26	0.83
2:P:361:HIS:H	2:P:361:HIS:CD2	1.97	0.82
1:D:165:GLN:H	1:D:165:GLN:NE2	1.76	0.82
1:F:165:GLN:H	1:F:165:GLN:CD	1.88	0.82
1:A:64:ARG:NH1	1:A:100:ASP:O	2.13	0.81
1:C:165:GLN:NE2	1:C:165:GLN:H	1.79	0.81
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.44	0.81
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.63	0.80
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.48	0.78
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.65	0.78
1:F:176:GLU:HG3	1:F:180:LYS:O	1.83	0.78
2:Q:429:CME:HE2	2:Q:438:SER:O	1.83	0.77
2:M:361:HIS:H	2:M:361:HIS:CD2	2.01	0.77
2:P:361:HIS:H	2:P:361:HIS:HD2	1.31	0.76
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.10	0.76
2:O:361:HIS:H	2:O:361:HIS:CD2	2.03	0.76
1:B:70:VAL:HG21	1:B:106:LEU:HD21	1.69	0.75
2:R:473:LYS:HD2	2:R:474:LEU:N	2.01	0.75
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.69	0.75
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.02	0.75
1:E:65:ASP:OD2	1:E:133:ARG:HD3	1.87	0.75
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.04	0.75
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.17	0.74
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.49	0.74
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.86	0.74
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.67	0.74
1:A:98:THR:HB	1:A:100:ASP:OD1	1.88	0.74
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.67	0.73
1:F:78:GLU:HG2	2:R:301:PRO:CB	2.18	0.73
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.73
1:C:41:LYS:NZ	1:C:86:GLU:O	2.22	0.73
1:D:24:GLU:OE1	1:D:25:ALA:N	2.21	0.73
2:R:364:LEU:HD22	2:R:440:ARG:CD	2.18	0.73
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.70	0.73
2:Q:522:ARG:NH1	5:Q:689:HOH:O	2.21	0.72
1:C:24:GLU:OE1	1:C:25:ALA:N	2.21	0.72
1:C:16:TYR:O	1:C:19:ILE:HG23	1.89	0.72
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.71	0.72
1:F:19:ILE:O	2:R:426:VAL:HG21	1.89	0.72
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.37	0.71
1:D:19:ILE:O	2:P:426:VAL:HG21	1.90	0.71
2:R:383:ARG:HG3	2:R:436:TYR:CE1	2.26	0.70
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.26	0.70
2:M:361:HIS:H	2:M:361:HIS:HD2	1.38	0.70
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.06	0.70
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.74	0.69
2:P:405:GLY:HA3	5:P:682:HOH:O	1.92	0.69
1:B:165:GLN:H	1:B:165:GLN:HE21	1.39	0.69
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.79	0.69
1:B:78:GLU:HG2	2:N:301:PRO:CB	2.22	0.69
2:R:522:ARG:HH21	2:R:524:ASP:CG	2.02	0.68
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.57	0.68
2:P:450:ARG:HD3	5:Q:622:HOH:O	1.93	0.68
1:F:78:GLU:HG2	2:R:301:PRO:HG3	1.76	0.68
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.24	0.67
1:B:165:GLN:NE2	1:B:165:GLN:N	2.38	0.67
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.30	0.67
1:A:24:GLU:CD	1:A:25:ALA:H	2.01	0.67
2:N:361:HIS:CD2	2:N:361:HIS:H	2.12	0.67
1:B:24:GLU:OE1	1:B:25:ALA:N	2.28	0.66
2:M:304:ASP:HB2	2:M:343:ILE:HG13	1.76	0.66
2:O:416:LEU:C	2:O:416:LEU:HD23	2.20	0.66
1:E:19:ILE:HD11	2:Q:408:TYR:HD2	1.61	0.66
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.30	0.66
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.31	0.66
1:C:143:LEU:HD23	1:C:143:LEU:C	2.22	0.65
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.11	0.65
2:R:416:LEU:C	2:R:416:LEU:HD23	2.21	0.65
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.79	0.65
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.27	0.65
1:F:24:GLU:HG3	5:F:781:HOH:O	1.96	0.65
1:A:176:GLU:HG3	1:A:180:LYS:O	1.96	0.65
2:P:442:ILE:O	2:P:442:ILE:HD12	1.97	0.65
2:Q:361:HIS:CG	2:Q:429:CME:HE3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:473:LYS:NZ	5:Q:675:HOH:O	2.23	0.65
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.27	0.65
1:F:165:GLN:NE2	1:F:165:GLN:N	2.44	0.64
1:B:176:GLU:HG3	1:B:180:LYS:O	1.96	0.64
1:F:98:THR:OG1	1:F:102:GLY:N	2.27	0.64
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.31	0.64
1:B:37:ASN:HB2	1:B:106:LEU:HD12	1.79	0.64
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.79	0.64
2:M:488:MET:HE1	2:P:508:LEU:HD23	1.78	0.64
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.12	0.64
1:D:176:GLU:HG3	1:D:180:LYS:O	1.98	0.64
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	1.98	0.64
2:P:313:ARG:O	2:P:318:LYS:HE2	1.97	0.63
1:F:100:ASP:CG	1:F:101:ALA:H	2.05	0.63
1:A:78:GLU:OE1	5:A:692:HOH:O	2.15	0.63
1:B:165:GLN:H	1:B:165:GLN:CD	2.04	0.63
2:P:359:HIS:O	2:P:366:ASN:HB3	1.98	0.63
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.99	0.63
1:D:35:ILE:HG21	1:D:92:PHE:HE1	1.64	0.63
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.99	0.63
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.81	0.63
1:C:24:GLU:CD	1:C:25:ALA:H	2.07	0.62
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.64	0.62
2:Q:447:TYR:HE1	4:Q:550:FHB:H5	1.64	0.62
1:F:163:GLN:CB	1:F:165:GLN:HE22	2.09	0.62
1:F:78:GLU:CG	2:R:301:PRO:HG3	2.30	0.62
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.00	0.62
1:B:78:GLU:HG2	2:N:301:PRO:CG	2.28	0.62
1:A:176:GLU:HA	1:A:180:LYS:O	1.99	0.62
1:B:180:LYS:HG2	1:B:181:THR:N	2.13	0.62
1:D:100:ASP:CG	1:D:101:ALA:H	2.07	0.62
1:B:165:GLN:HE21	1:B:165:GLN:N	1.97	0.61
2:Q:416:LEU:C	2:Q:416:LEU:CD2	2.73	0.61
2:Q:390:LYS:HD2	5:Q:667:HOH:O	2.00	0.61
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.35	0.61
2:N:359:HIS:O	2:N:366:ASN:HB3	2.00	0.61
1:C:24:GLU:OE1	1:C:25:ALA:HB2	2.00	0.61
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.30	0.61
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.83	0.61
2:Q:361:HIS:ND1	2:Q:429:CME:HE3	2.16	0.61
2:R:522:ARG:NH2	2:R:524:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:307:ARG:CG	2:N:533:THR:HG22	2.31	0.61
1:F:134:GLY:HA3	2:R:326:THR:HG22	1.83	0.60
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.36	0.60
1:F:116:ASN:OD1	1:F:116:ASN:C	2.44	0.60
2:R:408:TYR:HE2	2:R:447:TYR:CZ	2.19	0.60
1:E:98:THR:HB	1:E:100:ASP:OD1	2.00	0.60
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.00	0.60
2:N:390:LYS:HD2	5:N:749:HOH:O	2.00	0.60
2:M:359:HIS:O	2:M:366:ASN:HB3	2.01	0.60
2:O:478:LEU:HD23	2:O:478:LEU:C	2.27	0.60
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.82	0.60
1:F:24:GLU:OE1	1:F:25:ALA:N	2.35	0.60
2:M:473:LYS:NZ	5:M:710:HOH:O	2.31	0.60
1:C:164:PRO:HA	1:C:167:ARG:HD2	1.83	0.59
1:B:78:GLU:HG2	2:N:301:PRO:HB3	1.84	0.59
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.32	0.59
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.83	0.59
2:O:361:HIS:H	2:O:361:HIS:HD2	1.46	0.59
2:N:447:TYR:CE1	2:N:460:HIS:HE1	2.21	0.59
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.37	0.59
1:C:176:GLU:HG3	1:C:180:LYS:O	2.02	0.59
2:R:361:HIS:CD2	2:R:361:HIS:N	2.64	0.58
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.68	0.58
2:O:361:HIS:CG	2:O:429:CME:HE3	2.37	0.58
2:M:522:ARG:NH1	5:M:665:HOH:O	2.26	0.58
1:C:19:ILE:O	2:O:426:VAL:HG21	2.04	0.58
1:D:78:GLU:HG2	2:P:301:PRO:CB	2.34	0.58
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.86	0.58
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.85	0.58
2:O:376:GLU:O	2:O:442:ILE:HA	2.04	0.58
1:A:28:ASN:HB3	5:A:807:HOH:O	2.03	0.58
1:E:147:ASP:OD2	1:E:183:TYR:OH	2.18	0.58
2:N:376:GLU:O	2:N:442:ILE:HA	2.03	0.58
1:D:176:GLU:OE2	1:D:179:GLY:HA2	2.04	0.58
2:M:400:TRP:HA	2:M:425:GLY:O	2.04	0.57
1:C:165:GLN:H	1:C:165:GLN:HE21	1.51	0.57
1:A:100:ASP:CG	1:A:101:ALA:H	2.12	0.57
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.85	0.57
2:P:442:ILE:HD12	2:P:442:ILE:C	2.28	0.57
1:E:115:ASN:HA	1:E:121:PRO:HA	1.87	0.57
2:Q:487:PRO:O	2:Q:493:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.04	0.57
2:P:447:TYR:CE2	2:P:460:HIS:HE1	2.23	0.57
1:C:98:THR:O	1:C:102:GLY:HA2	2.05	0.57
1:A:24:GLU:OE1	1:A:25:ALA:HB2	2.05	0.56
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.40	0.56
1:E:66:SER:HB2	1:E:130:LEU:HD11	1.87	0.56
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.86	0.56
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.70	0.56
1:B:163:GLN:CB	1:B:165:GLN:HE22	2.13	0.56
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.70	0.56
1:B:132:ALA:HB3	1:B:135:ILE:HD12	1.88	0.56
1:D:165:GLN:HE21	1:D:165:GLN:N	1.95	0.56
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.31	0.56
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.86	0.56
1:C:50:LEU:O	1:C:182:ALA:HA	2.05	0.56
2:P:363:LEU:HD23	2:P:425:GLY:HA2	1.88	0.56
1:B:24:GLU:CD	1:B:25:ALA:H	2.14	0.56
2:N:478:LEU:HD12	2:N:523:PHE:CG	2.40	0.56
2:R:405:GLY:HA3	5:R:787:HOH:O	2.06	0.56
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.88	0.56
1:D:162:GLU:OE2	1:F:133:ARG:NH2	2.38	0.56
2:Q:447:TYR:CE1	4:Q:550:FHB:H5	2.40	0.56
1:D:98:THR:HB	1:D:100:ASP:OD1	2.06	0.56
1:E:78:GLU:HG2	2:Q:301:PRO:HB3	1.88	0.56
1:B:98:THR:O	1:B:102:GLY:HA2	2.06	0.55
1:F:50:LEU:O	1:F:182:ALA:HA	2.06	0.55
1:F:150:GLN:O	1:F:153:ALA:HB3	2.06	0.55
1:E:41:LYS:HD2	1:E:87:ASN:O	2.07	0.55
2:O:361:HIS:CD2	5:O:750:HOH:O	2.58	0.55
1:F:180:LYS:HG2	1:F:181:THR:N	2.22	0.55
1:D:143:LEU:C	1:D:143:LEU:HD23	2.32	0.55
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	1.89	0.55
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.32	0.55
1:F:174:ARG:HE	1:F:181:THR:CG2	2.20	0.55
1:F:131:PHE:O	1:F:132:ALA:HB2	2.05	0.55
1:E:98:THR:O	1:E:102:GLY:HA2	2.06	0.55
1:F:31:ARG:N	1:F:34:GLU:OE2	2.26	0.55
1:A:165:GLN:H	1:A:165:GLN:NE2	2.05	0.54
2:M:448:PRO:CB	2:P:516:MET:HA	2.36	0.54
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.89	0.54
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.71	0.54
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.73	0.54
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.89	0.54
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.07	0.54
2:R:307:ARG:CG	2:R:533:THR:HG22	2.38	0.54
1:B:19:ILE:O	2:N:426:VAL:HG21	2.07	0.54
2:Q:306:SER:CB	2:Q:530:GLN:HE21	2.20	0.54
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.23	0.53
1:A:165:GLN:H	1:A:165:GLN:CD	2.15	0.53
1:F:98:THR:O	1:F:102:GLY:HA2	2.08	0.53
1:A:41:LYS:HE3	1:A:87:ASN:O	2.09	0.53
1:A:69:GLU:OE1	2:M:473:LYS:HE2	2.07	0.53
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.43	0.53
2:M:399:MET:HE2	2:M:461:ILE:HG21	1.91	0.53
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.08	0.53
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.09	0.53
1:C:52:LEU:C	1:C:52:LEU:HD22	2.33	0.53
2:Q:364:LEU:HD11	2:Q:442:ILE:HG23	1.91	0.53
1:F:52:LEU:HD23	1:F:103:GLU:CD	2.34	0.53
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.72	0.53
1:D:52:LEU:C	1:D:52:LEU:HD22	2.34	0.53
2:Q:484:PRO:O	2:Q:488:MET:HE3	2.09	0.53
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.73	0.53
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.90	0.53
1:E:176:GLU:HA	1:E:180:LYS:O	2.09	0.53
1:C:67:PHE:C	1:C:68:LEU:HD12	2.34	0.53
2:O:486:ILE:N	2:O:487:PRO:HD2	2.24	0.53
2:N:307:ARG:NE	2:N:536:GLU:OE2	2.41	0.52
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.10	0.52
1:C:24:GLU:HG3	5:C:781:HOH:O	2.08	0.52
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.39	0.52
1:D:24:GLU:CD	1:D:25:ALA:H	2.17	0.52
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.90	0.52
1:E:32:ASP:HB2	5:E:810:HOH:O	2.08	0.52
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.44	0.52
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.90	0.52
2:P:416:LEU:C	2:P:416:LEU:HD23	2.35	0.52
1:F:19:ILE:O	2:R:426:VAL:CG2	2.56	0.52
2:R:383:ARG:HG3	2:R:436:TYR:CZ	2.43	0.52
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.44	0.52
2:P:484:PRO:O	2:P:488:MET:HE3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:PHE:O	1:E:132:ALA:HB2	2.08	0.52
1:F:24:GLU:CD	1:F:25:ALA:H	2.18	0.52
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.10	0.52
1:A:176:GLU:OE2	1:A:179:GLY:CA	2.56	0.52
2:M:376:GLU:OE1	5:M:635:HOH:O	2.19	0.52
1:F:64:ARG:HD3	1:F:99:PHE:O	2.10	0.52
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.90	0.52
2:P:376:GLU:O	2:P:442:ILE:HA	2.10	0.52
1:E:24:GLU:CD	1:E:25:ALA:H	2.17	0.52
1:E:50:LEU:O	1:E:182:ALA:HA	2.10	0.52
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.28	0.52
2:M:465:ILE:N	2:M:465:ILE:HD12	2.25	0.52
2:N:447:TYR:HB2	2:N:448:PRO:HD2	1.92	0.51
1:E:24:GLU:O	1:E:27:GLY:N	2.42	0.51
1:B:143:LEU:C	1:B:143:LEU:HD23	2.35	0.51
2:R:447:TYR:CE2	4:R:550:FHB:H5	2.45	0.51
2:M:405:GLY:HA3	5:M:643:HOH:O	2.10	0.51
2:O:416:LEU:C	2:O:416:LEU:CD2	2.84	0.51
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.10	0.51
1:E:143:LEU:HD23	1:E:143:LEU:C	2.35	0.51
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.92	0.51
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.92	0.51
1:C:131:PHE:O	1:C:132:ALA:HB2	2.11	0.51
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.92	0.51
2:R:306:SER:CB	2:R:530:GLN:HE21	2.23	0.51
1:E:70:VAL:HG12	1:E:128:ILE:HG12	1.92	0.51
1:F:84:ASN:O	1:F:87:ASN:HB2	2.10	0.51
1:F:18:HIS:HE1	1:F:99:PHE:HE1	1.51	0.51
2:R:314:ASN:OD1	2:R:318:LYS:HE2	2.11	0.51
2:M:376:GLU:HG2	2:P:446:PRO:HD2	1.92	0.51
2:Q:399:MET:HA	2:Q:462:HIS:O	2.11	0.51
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.26	0.51
1:D:19:ILE:HG13	2:P:400:TRP:HB2	1.91	0.51
1:D:38:ARG:HG3	1:D:107:HIS:HB2	1.91	0.51
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.40	0.51
2:Q:517:ASP:OD1	2:Q:517:ASP:C	2.54	0.51
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.93	0.50
1:D:36:TRP:CG	1:D:37:ASN:H	2.29	0.50
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.50
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.94	0.50
2:O:429:CME:HE2	2:O:438:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:HG12	2:O:400:TRP:HB2	1.92	0.50
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.47	0.50
1:C:68:LEU:HD12	1:C:68:LEU:N	2.27	0.50
1:D:35:ILE:HG21	1:D:92:PHE:CE1	2.44	0.50
1:F:49:ILE:CA	1:F:180:LYS:HE2	2.41	0.50
2:Q:460:HIS:HA	2:Q:478:LEU:O	2.11	0.50
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.47	0.50
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.42	0.50
2:M:447:TYR:HB2	2:M:448:PRO:HD2	1.94	0.50
2:O:359:HIS:O	2:O:366:ASN:HB3	2.12	0.50
1:F:180:LYS:CG	1:F:181:THR:N	2.75	0.50
2:R:361:HIS:CG	2:R:429:CME:HE3	2.47	0.50
1:E:199:ASP:CG	2:Q:313:ARG:HE	2.19	0.50
1:A:24:GLU:OE1	1:A:25:ALA:N	2.45	0.49
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.93	0.49
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.93	0.49
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.46	0.49
2:N:534:HIS:CE1	2:P:512:ASN:O	2.65	0.49
1:F:24:GLU:OE1	1:F:25:ALA:HB2	2.12	0.49
1:F:143:LEU:C	1:F:143:LEU:HD23	2.36	0.49
1:A:114:VAL:HG22	1:A:122:MET:HE3	1.94	0.49
2:M:510:MET:HE1	2:P:456:TRP:CD1	2.48	0.49
1:D:50:LEU:O	1:D:182:ALA:HA	2.12	0.49
1:F:184:ARG:NH1	1:F:184:ARG:HG3	2.26	0.49
1:A:98:THR:OG1	1:A:102:GLY:N	2.44	0.49
2:N:410:HIS:O	5:N:855:HOH:O	2.19	0.49
1:D:98:THR:OG1	1:D:102:GLY:N	2.37	0.49
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.47	0.49
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.93	0.49
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.47	0.49
1:E:180:LYS:HG2	1:E:181:THR:N	2.27	0.49
2:R:392:VAL:HG12	2:R:395:THR:HB	1.94	0.49
2:M:392:VAL:HG12	2:M:395:THR:HB	1.94	0.49
2:M:478:LEU:HD23	2:M:478:LEU:C	2.37	0.49
1:D:84:ASN:OD1	1:D:86:GLU:HB2	2.12	0.49
1:E:24:GLU:OE1	1:E:25:ALA:N	2.36	0.49
1:E:69:GLU:OE1	2:Q:473:LYS:HE2	2.12	0.49
2:M:448:PRO:HB2	2:P:516:MET:HA	1.94	0.49
2:N:362:ASP:OD2	2:N:440:ARG:NH1	2.45	0.49
2:Q:390:LYS:HD3	5:Q:745:HOH:O	2.12	0.49
2:R:371:GLY:N	2:R:422:ASN:ND2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD12	1:B:51:LEU:N	2.27	0.49
1:D:133:ARG:HG3	2:P:326:THR:HG21	1.95	0.49
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.47	0.49
2:O:381:ALA:O	2:O:522:ARG:HA	2.13	0.49
1:D:27:GLY:HA3	2:P:411:LYS:HE3	1.95	0.49
1:E:174:ARG:HE	1:E:181:THR:HG23	1.78	0.49
1:C:165:GLN:HE21	1:C:165:GLN:N	2.11	0.48
1:E:176:GLU:HG3	1:E:180:LYS:O	2.13	0.48
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.13	0.48
1:F:125:HIS:HA	1:F:143:LEU:O	2.12	0.48
2:R:361:HIS:ND1	2:R:429:CME:HE3	2.27	0.48
2:R:447:TYR:HE2	4:R:550:FHB:H5	1.78	0.48
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.31	0.48
1:E:37:ASN:HB2	1:E:106:LEU:HD12	1.95	0.48
2:R:400:TRP:HA	2:R:425:GLY:O	2.12	0.48
2:R:531:ARG:NH1	2:R:532:LYS:O	2.44	0.48
1:F:49:ILE:HA	1:F:180:LYS:HE2	1.94	0.48
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.94	0.48
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.94	0.48
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.96	0.48
1:C:78:GLU:HG2	2:O:301:PRO:CB	2.44	0.48
2:N:447:TYR:CE1	2:N:460:HIS:CE1	3.01	0.48
1:C:180:LYS:HG2	1:C:181:THR:N	2.28	0.48
2:M:364:LEU:HB2	2:M:440:ARG:HD3	1.94	0.48
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.49	0.48
1:D:24:GLU:O	1:D:27:GLY:N	2.42	0.48
1:D:116:ASN:OD1	1:D:116:ASN:C	2.57	0.48
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.75	0.47
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.95	0.47
1:F:165:GLN:CD	1:F:165:GLN:N	2.66	0.47
2:R:363:LEU:N	2:R:363:LEU:HD12	2.29	0.47
2:N:392:VAL:HG12	2:N:395:THR:HB	1.96	0.47
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.94	0.47
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.95	0.47
2:Q:447:TYR:CE2	2:Q:460:HIS:HE1	2.33	0.47
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.95	0.47
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.96	0.47
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.14	0.47
1:F:171:ILE:HD12	1:F:171:ILE:N	2.29	0.47
1:B:176:GLU:HG3	1:B:180:LYS:C	2.39	0.47
2:P:408:TYR:HE2	2:P:447:TYR:CZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:THR:OG1	1:F:101:ALA:HB3	2.14	0.47
1:F:116:ASN:OD1	1:F:118:ALA:N	2.48	0.47
2:R:437:TYR:CD1	2:R:437:TYR:C	2.92	0.47
1:C:78:GLU:HG2	2:O:301:PRO:HG3	1.96	0.47
1:C:114:VAL:HG23	1:C:122:MET:CE	2.41	0.47
1:D:78:GLU:HG2	2:P:301:PRO:HB3	1.95	0.47
1:B:50:LEU:O	1:B:182:ALA:HA	2.15	0.47
2:N:399:MET:HA	2:N:462:HIS:O	2.15	0.47
1:D:58:GLY:HA2	1:D:190:GLN:HB3	1.96	0.47
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.15	0.47
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.96	0.47
1:D:32:ASP:HB2	5:P:765:HOH:O	2.14	0.47
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.49	0.47
1:E:53:GLY:O	1:E:103:GLU:HG3	2.15	0.47
1:F:50:LEU:HD12	1:F:51:LEU:N	2.30	0.47
2:R:390:LYS:HE2	5:R:864:HOH:O	2.15	0.47
1:C:174:ARG:HE	1:C:181:THR:HG23	1.80	0.46
2:P:400:TRP:HA	2:P:425:GLY:O	2.15	0.46
2:Q:450:ARG:HD3	5:R:739:HOH:O	2.15	0.46
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.38	0.46
1:C:41:LYS:NZ	1:C:86:GLU:C	2.72	0.46
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.81	0.46
1:E:70:VAL:HG21	1:E:106:LEU:HD21	1.96	0.46
2:R:416:LEU:C	2:R:416:LEU:CD2	2.88	0.46
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.50	0.46
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.78	0.46
2:M:484:PRO:O	2:M:488:MET:HE3	2.15	0.46
2:N:416:LEU:HD23	2:N:416:LEU:C	2.41	0.46
1:E:24:GLU:HG3	5:E:781:HOH:O	2.15	0.46
2:M:385:VAL:O	2:M:526:VAL:HA	2.16	0.46
2:P:484:PRO:O	2:P:487:PRO:HD2	2.16	0.46
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.76	0.46
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.98	0.46
1:C:165:GLN:H	1:C:165:GLN:CD	2.16	0.46
2:P:307:ARG:HD2	5:P:693:HOH:O	2.15	0.46
1:B:1:PRO:HB3	2:P:508:LEU:HB3	1.97	0.46
2:O:478:LEU:HD12	2:O:523:PHE:CD2	2.50	0.46
1:C:36:TRP:CG	1:C:37:ASN:H	2.33	0.46
2:P:447:TYR:CE2	2:P:460:HIS:CE1	3.03	0.46
1:C:131:PHE:CD2	2:O:475:ILE:HD12	2.51	0.46
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.77	0.46
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.16	0.46
2:O:447:TYR:HE1	4:O:550:FHB:H5	1.80	0.46
1:A:143:LEU:C	1:A:143:LEU:HD23	2.41	0.45
2:M:481:GLU:CD	1:E:1:PRO:H3	2.23	0.45
1:C:38:ARG:HH11	1:C:38:ARG:HD2	1.63	0.45
1:F:143:LEU:HD23	1:F:144:TYR:N	2.32	0.45
2:R:383:ARG:HA	2:R:435:GLY:O	2.16	0.45
1:B:199:ASP:CG	2:N:313:ARG:HE	2.25	0.45
2:P:448:PRO:HD3	2:P:456:TRP:CZ3	2.51	0.45
1:E:52:LEU:C	1:E:52:LEU:HD22	2.41	0.45
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.96	0.45
1:F:176:GLU:HG3	1:F:180:LYS:C	2.41	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.74	0.45
1:C:12:THR:HG21	2:O:324:TYR:OH	2.16	0.45
2:N:400:TRP:HA	2:N:425:GLY:O	2.17	0.45
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.79	0.45
1:E:100:ASP:CG	1:E:101:ALA:H	2.25	0.45
2:R:383:ARG:HB2	2:R:522:ARG:NH2	2.32	0.45
2:M:434:ASP:HB2	2:M:436:TYR:HD2	1.82	0.45
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	3.05	0.45
2:Q:448:PRO:HD3	2:Q:456:TRP:CZ3	2.51	0.45
1:F:115:ASN:HA	1:F:121:PRO:HA	1.99	0.45
2:N:364:LEU:HD12	2:N:373:PRO:HG2	1.98	0.45
2:M:483:ASP:HA	2:M:484:PRO:HD2	1.81	0.45
1:B:174:ARG:HE	1:B:181:THR:HG23	1.82	0.45
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.82	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.41	0.45
2:N:493:LYS:HE3	2:N:493:LYS:HB2	1.73	0.45
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.52	0.45
2:N:534:HIS:HE1	2:P:512:ASN:O	2.00	0.45
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.79	0.45
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.17	0.45
1:F:131:PHE:CE2	2:R:475:ILE:HD12	2.51	0.45
2:R:416:LEU:HD23	2:R:417:ALA:N	2.32	0.45
1:B:24:GLU:O	1:B:27:GLY:N	2.45	0.44
2:N:447:TYR:HE1	2:N:460:HIS:CE1	2.36	0.44
2:N:522:ARG:NH1	5:N:774:HOH:O	2.15	0.44
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.16	0.44
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.17	0.44
2:R:385:VAL:O	2:R:526:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:HG3	5:A:781:HOH:O	2.16	0.44
2:M:517:ASP:C	2:M:517:ASP:OD1	2.60	0.44
2:N:408:TYR:HE1	2:N:447:TYR:CZ	2.35	0.44
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.82	0.44
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.49	0.44
5:E:697:HOH:O	2:Q:426:VAL:HG21	2.17	0.44
1:F:146:ASP:HB3	1:F:171:ILE:CG2	2.47	0.44
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.71	0.44
1:B:28:ASN:HB3	1:B:29:PRO:HD2	1.98	0.44
2:Q:390:LYS:HD3	5:Q:725:HOH:O	2.16	0.44
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.82	0.44
2:R:302:ALA:HB1	2:R:347:THR:CG2	2.47	0.44
2:N:312:ASP:OD1	2:N:312:ASP:C	2.61	0.44
1:C:19:ILE:HD13	1:C:19:ILE:HG21	1.60	0.44
2:O:407:ARG:HD3	2:O:417:ALA:O	2.17	0.44
2:Q:383:ARG:HA	2:Q:435:GLY:O	2.18	0.44
2:R:350:ASN:OD1	2:R:350:ASN:C	2.60	0.44
2:R:473:LYS:HD2	2:R:474:LEU:H	1.78	0.44
1:A:199:ASP:CG	2:M:313:ARG:HE	2.26	0.44
1:B:4:LEU:HD22	2:P:511:ASN:CG	2.43	0.44
2:M:512:ASN:O	2:Q:534:HIS:HE1	2.00	0.44
2:P:341:GLN:HB3	2:P:346:THR:CG2	2.48	0.44
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.99	0.44
1:F:122:MET:HG2	1:F:156:PRO:HG2	1.99	0.44
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.18	0.44
2:N:373:PRO:HB3	2:N:423:PHE:HB2	2.00	0.44
1:D:52:LEU:C	1:D:52:LEU:CD2	2.91	0.44
2:R:304:ASP:HA	5:R:876:HOH:O	2.18	0.44
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.90	0.44
2:R:411:LYS:O	2:R:414:ARG:NH2	2.49	0.44
1:D:100:ASP:CG	1:D:101:ALA:N	2.76	0.44
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.33	0.44
1:A:35:ILE:HG21	1:A:92:PHE:HE1	1.82	0.43
1:D:33:GLN:HG2	1:D:85:LEU:HD12	2.00	0.43
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.35	0.43
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.53	0.43
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.51	0.43
1:C:64:ARG:HD3	1:C:99:PHE:O	2.18	0.43
2:O:411:LYS:O	2:O:414:ARG:NH2	2.51	0.43
2:O:437:TYR:CD1	2:O:437:TYR:C	2.96	0.43
1:D:3:GLU:HA	1:D:3:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:489:CYS:C	2:P:493:LYS:HE3	2.44	0.43
2:P:497:ASN:OD1	2:P:499:GLU:HB2	2.18	0.43
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	2.00	0.43
1:F:47:GLU:O	1:F:49:ILE:HG23	2.18	0.43
2:R:408:TYR:HE2	2:R:447:TYR:CE1	2.35	0.43
2:R:447:TYR:CE1	2:R:460:HIS:HE1	2.36	0.43
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.83	0.43
2:O:405:GLY:HA3	5:O:682:HOH:O	2.18	0.43
2:Q:390:LYS:HG2	2:Q:391:PRO:O	2.18	0.43
2:R:372:LEU:HA	2:R:373:PRO:HD3	1.91	0.43
1:B:7:GLU:CD	2:N:316:HIS:HE2	2.26	0.43
1:C:78:GLU:CG	2:O:301:PRO:HG3	2.48	0.43
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.47	0.43
1:C:73:ALA:HB1	1:C:78:GLU:N	2.34	0.43
2:Q:350:ASN:C	2:Q:350:ASN:OD1	2.60	0.43
1:F:134:GLY:HA3	2:R:326:THR:CG2	2.48	0.43
2:M:362:ASP:CG	2:M:440:ARG:HD2	2.43	0.43
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.32	0.43
2:N:356:PHE:CE2	2:N:428:ARG:HD3	2.54	0.43
1:C:123:ALA:HB3	1:C:144:TYR:CE2	2.53	0.43
2:P:381:ALA:O	2:P:522:ARG:HA	2.18	0.43
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.73	0.43
1:E:15:PRO:HB3	1:E:133:ARG:HD2	2.01	0.43
1:E:58:GLY:HA2	1:E:190:GLN:HB3	2.01	0.43
2:M:399:MET:HE2	2:M:461:ILE:CG2	2.48	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.01	0.43
1:F:98:THR:HB	1:F:100:ASP:OD1	2.18	0.43
2:R:447:TYR:HB2	2:R:448:PRO:HD2	2.00	0.43
2:O:522:ARG:NH1	5:O:716:HOH:O	2.24	0.43
1:C:24:GLU:OE1	1:C:25:ALA:CB	2.64	0.43
2:P:437:TYR:CD1	2:P:437:TYR:C	2.97	0.43
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.54	0.43
2:Q:441:THR:OG1	2:Q:442:ILE:N	2.51	0.43
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.55	0.42
2:N:405:GLY:HA3	5:N:752:HOH:O	2.19	0.42
1:D:78:GLU:HG2	2:P:301:PRO:HG2	2.01	0.42
2:P:318:LYS:HA	2:P:318:LYS:HD3	1.74	0.42
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.77	0.42
1:F:77:GLY:O	1:F:114:VAL:HG12	2.19	0.42
2:R:395:THR:O	2:R:430:LEU:HA	2.19	0.42
1:B:38:ARG:HA	1:B:107:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.80	0.42
2:Q:408:TYR:CE1	2:Q:447:TYR:CE2	3.06	0.42
1:F:31:ARG:HH11	2:R:428:ARG:HG2	1.80	0.42
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.67	0.42
2:R:386:ASP:HA	2:R:527:LEU:O	2.19	0.42
1:C:11:GLN:HB2	2:O:477:GLN:HG3	2.00	0.42
2:N:383:ARG:HA	2:N:435:GLY:O	2.20	0.42
1:C:78:GLU:HG2	2:O:301:PRO:HB3	2.00	0.42
2:O:447:TYR:CE1	4:O:550:FHB:H5	2.55	0.42
1:D:168:GLU:HA	1:D:171:ILE:HD12	2.00	0.42
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.42
1:C:41:LYS:HZ2	1:C:86:GLU:C	2.28	0.42
1:D:98:THR:O	1:D:102:GLY:HA2	2.19	0.42
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.90	0.42
1:F:23:LEU:O	1:F:24:GLU:C	2.63	0.42
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.69	0.42
1:A:54:GLN:HG2	1:A:102:GLY:O	2.18	0.42
1:C:176:GLU:HG3	1:C:180:LYS:C	2.45	0.42
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.79	0.42
1:D:52:LEU:HD21	1:D:184:ARG:NH1	2.34	0.42
2:P:468:PRO:HD2	2:P:472:THR:HG21	2.00	0.42
2:Q:405:GLY:HA3	5:Q:670:HOH:O	2.18	0.42
1:A:176:GLU:HG3	1:A:180:LYS:C	2.44	0.42
1:E:72:GLN:HB3	1:E:126:ILE:HG12	2.01	0.42
1:B:19:ILE:O	2:N:426:VAL:CG2	2.67	0.42
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.54	0.42
2:Q:437:TYR:CD1	2:Q:437:TYR:C	2.98	0.42
1:A:51:LEU:HD12	1:A:106:LEU:HD23	2.01	0.41
2:M:515:PRO:HB3	2:P:453:PRO:O	2.20	0.41
1:B:84:ASN:OD1	1:B:86:GLU:HB2	2.20	0.41
1:D:24:GLU:HG3	5:D:781:HOH:O	2.19	0.41
2:M:364:LEU:HD11	2:M:442:ILE:HG23	2.02	0.41
1:B:131:PHE:O	1:B:132:ALA:HB2	2.20	0.41
2:N:325:LYS:HG2	2:O:335:ALA:HB1	2.02	0.41
2:N:361:HIS:H	2:N:361:HIS:HD2	1.61	0.41
2:Q:315:TRP:CZ2	2:Q:500:ALA:HA	2.55	0.41
2:Q:363:LEU:HD23	2:Q:425:GLY:CA	2.48	0.41
2:R:364:LEU:CD2	2:R:440:ARG:HD3	2.38	0.41
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.50	0.41
2:O:483:ASP:HA	2:O:484:PRO:HD2	1.94	0.41
1:E:19:ILE:HG21	2:Q:410:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:321:THR:HG21	2:R:494:SER:HB2	2.02	0.41
2:M:376:GLU:O	2:M:442:ILE:HA	2.21	0.41
2:N:333:ARG:HD3	2:N:333:ARG:HA	1.95	0.41
2:N:363:LEU:HD11	2:N:427:GLY:HA3	2.02	0.41
2:N:478:LEU:HD12	2:N:523:PHE:CD2	2.55	0.41
1:C:38:ARG:HG3	1:C:107:HIS:HB2	2.02	0.41
1:D:176:GLU:HG2	1:D:179:GLY:CA	2.50	0.41
2:R:447:TYR:CE1	2:R:460:HIS:CE1	3.09	0.41
2:M:449:TRP:CZ3	2:M:451:ASN:HB2	2.55	0.41
1:D:51:LEU:HB2	1:D:106:LEU:HB3	2.03	0.41
1:B:114:VAL:CG2	1:B:122:MET:HE3	2.51	0.41
2:N:306:SER:O	2:N:307:ARG:NH1	2.53	0.41
1:C:98:THR:OG1	1:C:101:ALA:HB3	2.20	0.41
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.33	0.41
1:E:114:VAL:HG23	1:E:122:MET:CE	2.51	0.41
1:C:100:ASP:OD1	1:C:100:ASP:N	2.45	0.41
2:O:408:TYR:HE1	2:O:447:TYR:CZ	2.39	0.41
1:D:19:ILE:HG22	1:D:26:ALA:HB1	2.02	0.41
2:P:416:LEU:C	2:P:416:LEU:CD2	2.94	0.41
1:F:52:LEU:C	1:F:52:LEU:HD22	2.46	0.41
2:M:493:LYS:C	2:M:495:ILE:N	2.76	0.41
1:B:24:GLU:HG3	5:B:781:HOH:O	2.20	0.41
1:B:62:LEU:HD12	1:B:64:ARG:NH2	2.35	0.41
5:B:697:HOH:O	2:N:426:VAL:HG21	2.21	0.41
1:C:140:HIS:O	1:C:197:PHE:HA	2.20	0.41
1:D:4:LEU:HB3	2:P:387:GLN:HB3	2.01	0.41
1:E:19:ILE:HG23	2:Q:410:HIS:HD2	1.86	0.41
1:E:24:GLU:OE1	1:E:25:ALA:CB	2.69	0.41
1:E:146:ASP:HB3	1:E:171:ILE:HG22	2.03	0.41
1:F:155:CYS:O	1:F:159:ASN:ND2	2.46	0.41
1:E:36:TRP:CG	1:E:37:ASN:H	2.39	0.41
2:R:364:LEU:HB2	2:R:440:ARG:HD3	2.03	0.41
1:A:68:LEU:N	1:A:68:LEU:HD12	2.37	0.40
1:A:180:LYS:CG	1:A:181:THR:N	2.84	0.40
1:C:163:GLN:CB	1:C:165:GLN:HE22	2.33	0.40
2:O:497:ASN:HB2	5:O:792:HOH:O	2.21	0.40
2:P:420:ASP:HA	2:P:421:PRO:HD2	1.93	0.40
1:F:36:TRP:CG	1:F:37:ASN:H	2.40	0.40
2:M:304:ASP:HB2	2:M:343:ILE:CG1	2.48	0.40
2:M:456:TRP:CG	2:P:519:LEU:HD21	2.56	0.40
2:P:333:ARG:HD3	2:P:333:ARG:HA	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LEU:HA	1:E:104:TRP:O	2.21	0.40
2:Q:468:PRO:HD2	2:Q:472:THR:HG21	2.03	0.40
2:N:383:ARG:NE	2:N:434:ASP:O	2.47	0.40
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.90	0.40
1:E:54:GLN:OE1	1:E:184:ARG:NH2	2.54	0.40
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.37	0.40
2:P:308:PHE:HA	2:P:529:GLY:O	2.22	0.40
1:A:20:GLY:C	1:A:21:LEU:HD23	2.47	0.40
1:A:176:GLU:HG2	1:A:179:GLY:HA2	2.04	0.40
2:N:448:PRO:HD3	2:N:456:TRP:CZ3	2.57	0.40
1:D:78:GLU:CD	2:P:301:PRO:HG2	2.46	0.40
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.57	0.40
1:F:12:THR:HA	1:F:135:ILE:O	2.21	0.40
1:F:113:VAL:HA	5:F:680:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	F	198/200 (99%)	185 (93%)	13 (7%)	0	100	100
2	M	228/238 (96%)	218 (96%)	10 (4%)	0	100	100
2	N	228/238 (96%)	221 (97%)	7 (3%)	0	100	100
2	O	228/238 (96%)	220 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	Q	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	R	228/238 (96%)	218 (96%)	10 (4%)	0	100	100
All	All	2556/2628 (97%)	2454 (96%)	102 (4%)	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	24
1	B	162/163 (99%)	152 (94%)	10 (6%)	16	12
1	C	162/163 (99%)	154 (95%)	8 (5%)	22	19
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	19
1	E	162/163 (99%)	153 (94%)	9 (6%)	19	15
1	F	162/163 (99%)	156 (96%)	6 (4%)	30	30
2	M	195/201 (97%)	185 (95%)	10 (5%)	21	18
2	N	195/201 (97%)	187 (96%)	8 (4%)	27	26
2	O	195/201 (97%)	186 (95%)	9 (5%)	24	22
2	P	195/201 (97%)	190 (97%)	5 (3%)	40	43
2	Q	195/201 (97%)	189 (97%)	6 (3%)	35	37
2	R	195/201 (97%)	188 (96%)	7 (4%)	31	31
All	All	2142/2184 (98%)	2049 (96%)	93 (4%)	26	24

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE

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Mol	Chain	Res	Type
1	A	24	GLU
1	A	52	LEU
1	A	114	VAL
1	A	143	LEU
1	A	165	GLN
2	M	343	ILE
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	433	SER
2	M	440	ARG
2	M	450	ARG
2	M	473	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	24	GLU
1	B	32	ASP
1	B	52	LEU
1	B	78	GLU
1	B	143	LEU
1	B	158	LEU
1	B	165	GLN
1	B	176	GLU
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	428	ARG
2	N	450	ARG
2	N	505	ILE
1	C	4	LEU
1	C	19	ILE
1	C	24	GLU
1	C	52	LEU
1	C	100	ASP
1	C	141	THR
1	C	143	LEU
1	C	165	GLN
2	O	326	THR

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Mol	Chain	Res	Type
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	399	MET
2	O	416	LEU
2	O	428	ARG
2	O	450	ARG
2	O	478	LEU
1	D	4	LEU
1	D	24	GLU
1	D	43	ASP
1	D	52	LEU
1	D	114	VAL
1	D	126	ILE
1	D	164	PRO
1	D	165	GLN
2	P	372	LEU
2	P	395	THR
2	P	416	LEU
2	P	450	ARG
2	P	478	LEU
1	E	4	LEU
1	E	19	ILE
1	E	24	GLU
1	E	38	ARG
1	E	52	LEU
1	E	68	LEU
1	E	165	GLN
1	E	168	GLU
1	E	184	ARG
2	Q	372	LEU
2	Q	390	LYS
2	Q	395	THR
2	Q	416	LEU
2	Q	491	ILE
2	Q	505	ILE
1	F	4	LEU
1	F	19	ILE
1	F	24	GLU
1	F	52	LEU
1	F	143	LEU
1	F	165	GLN

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Mol	Chain	Res	Type
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	440	ARG
2	R	450	ARG
2	R	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	165	GLN
2	M	314	ASN
2	M	361	HIS
2	M	412	ASN
1	B	165	GLN
2	N	305	ASN
2	N	359	HIS
2	N	361	HIS
2	N	412	ASN
2	N	530	GLN
1	C	28	ASN
1	C	87	ASN
1	C	127	ASN
1	C	163	GLN
1	C	165	GLN
2	O	305	ASN
2	O	361	HIS
2	O	394	ASN
2	O	412	ASN
2	O	530	GLN
1	D	115	ASN
1	D	127	ASN
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	394	ASN
2	P	412	ASN
1	E	11	GLN
1	E	163	GLN
1	E	165	GLN

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Mol	Chain	Res	Type
2	Q	361	HIS
2	Q	530	GLN
1	F	59	ASN
1	F	140	HIS
1	F	150	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	422	ASN
2	R	503	GLN
2	R	530	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	0.81	0	6,9,11	1.25	1 (16%)
2	CME	P	429	2	8,9,10	0.84	0	6,9,11	1.03	0
2	CME	O	429	2	8,9,10	0.81	0	6,9,11	1.13	0
2	CME	M	429	2	8,9,10	0.80	0	6,9,11	0.66	0
2	CME	R	429	2	8,9,10	0.94	0	6,9,11	1.34	0
2	CME	N	429	2	8,9,10	0.74	0	6,9,11	0.61	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	P	429	2	-	1/5/8/10	-
2	CME	O	429	2	-	1/5/8/10	-
2	CME	M	429	2	-	1/5/8/10	-
2	CME	R	429	2	-	1/5/8/10	-
2	CME	N	429	2	-	0/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	Q	429	CME	CZ-CE-SD	-2.36	105.51	113.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	429	CME	3	0
2	O	429	CME	2	0
2	R	429	CME	2	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	FHB	N	550	3	11,11,11	1.29	1 (9%)	13,15,15	0.75	0
4	FHB	M	550	3	11,11,11	1.33	1 (9%)	13,15,15	1.11	2 (15%)
4	FHB	Q	551	-	11,11,11	1.11	0	13,15,15	1.06	1 (7%)
4	FHB	P	551	-	11,11,11	1.26	1 (9%)	13,15,15	1.21	1 (7%)
4	FHB	O	551	-	11,11,11	1.13	0	13,15,15	0.93	0
4	FHB	M	551	-	11,11,11	1.26	1 (9%)	13,15,15	1.07	2 (15%)
4	FHB	Q	550	3	11,11,11	1.49	2 (18%)	13,15,15	0.98	0
4	FHB	N	551	-	11,11,11	1.14	1 (9%)	13,15,15	1.14	2 (15%)
4	FHB	R	551	-	11,11,11	1.10	0	13,15,15	1.01	1 (7%)
4	FHB	P	550	3	11,11,11	1.26	1 (9%)	13,15,15	1.14	2 (15%)
4	FHB	O	550	3	11,11,11	1.27	2 (18%)	13,15,15	0.94	0
4	FHB	R	550	3	11,11,11	1.06	1 (9%)	13,15,15	1.00	1 (7%)

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	FHB	N	550	3	-	0/4/4/4	0/1/1/1
4	FHB	M	550	3	-	0/4/4/4	0/1/1/1
4	FHB	Q	551	-	-	0/4/4/4	0/1/1/1
4	FHB	P	551	-	-	0/4/4/4	0/1/1/1
4	FHB	O	551	-	-	0/4/4/4	0/1/1/1
4	FHB	M	551	-	-	0/4/4/4	0/1/1/1
4	FHB	Q	550	3	-	0/4/4/4	0/1/1/1
4	FHB	N	551	-	-	0/4/4/4	0/1/1/1
4	FHB	R	551	-	-	0/4/4/4	0/1/1/1
4	FHB	P	550	3	-	0/4/4/4	0/1/1/1
4	FHB	O	550	3	-	0/4/4/4	0/1/1/1
4	FHB	R	550	3	-	0/4/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	550	FHB	C2-C1	2.93	1.43	1.39
4	M	550	FHB	O2-C7	-2.90	1.21	1.30
4	N	550	FHB	O2-C7	-2.80	1.22	1.30
4	O	550	FHB	C4-C3	2.71	1.41	1.39
4	Q	550	FHB	O2-C7	-2.67	1.22	1.30
4	R	550	FHB	O2-C7	-2.35	1.23	1.30
4	N	551	FHB	O2-C7	-2.24	1.23	1.30
4	O	550	FHB	O2-C7	-2.10	1.24	1.30
4	P	551	FHB	C4-C3	2.10	1.40	1.39
4	M	551	FHB	C6-C1	2.09	1.42	1.39
4	P	550	FHB	O2-C7	-2.05	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	551	FHB	O2-C7-C1	2.74	121.88	114.84
4	N	551	FHB	O2-C7-C1	2.56	121.41	114.84
4	P	550	FHB	O2-C7-C1	2.50	121.25	114.84
4	M	551	FHB	O2-C7-C1	2.45	121.12	114.84
4	R	550	FHB	O2-C7-O1	-2.34	118.33	123.35
4	M	551	FHB	O2-C7-O1	-2.31	118.38	123.35
4	M	550	FHB	O2-C7-O1	-2.18	118.67	123.35
4	N	551	FHB	O2-C7-O1	-2.18	118.67	123.35
4	R	551	FHB	O2-C7-C1	2.18	120.43	114.84
4	Q	551	FHB	O2-C7-O1	-2.12	118.80	123.35
4	P	550	FHB	O2-C7-O1	-2.10	118.83	123.35
4	M	550	FHB	O2-C7-C1	2.08	120.18	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	550	FHB	2	0
4	O	550	FHB	2	0
4	R	550	FHB	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.