



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:06 am BST

PDB ID : 3PCJ
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 2-HYDROXYISONICOTINIC ACID N-OXIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.13 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

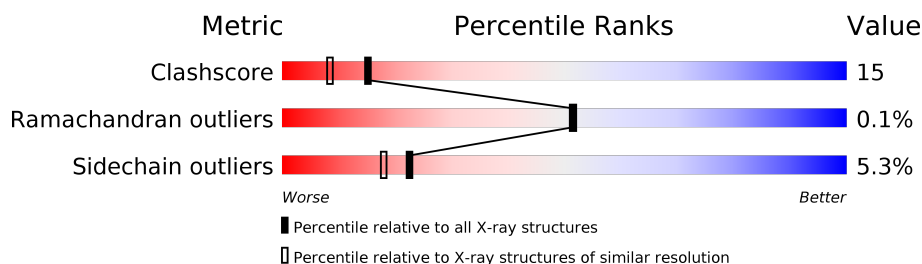
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)





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 on 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	69% 24% 7% .
1	B	200	68% 29% . .
1	C	200	66% 29% 5% .
1	D	200	72% 22% 6% .
1	E	200	60% 34% 6% .
1	F	200	58% 36% 6% .
2	M	238	71% 23% . . .
2	N	238	71% 22% 5% .

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Mol	Chain	Length	Quality of chain
2	O	238	 65%26%7% •
2	P	238	 69%23%5% • •
2	Q	238	 67%25%5% •
2	R	238	 61%29%7% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21978 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.

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			

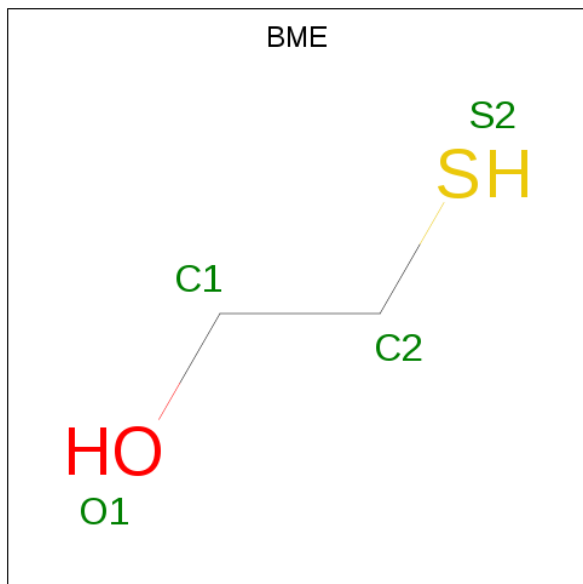
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	N	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	O	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	P	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	R	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

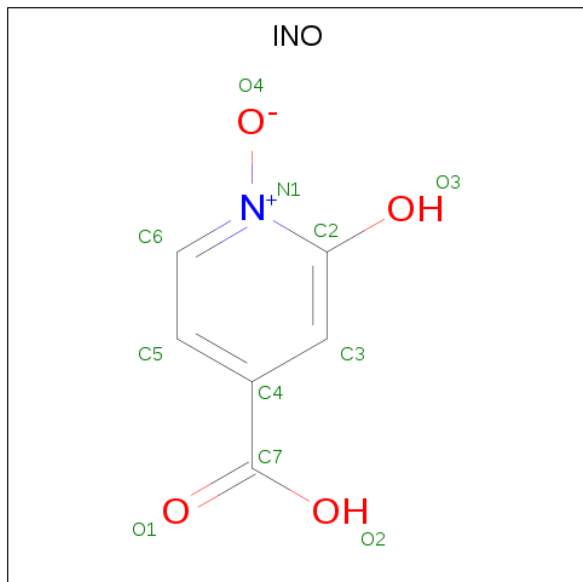
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 2-HYDROXYISONICOTINIC ACID N-OXIDE (three-letter code: INO) (formula: C₆H₅NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			11	6	1	4		
5	N	1	Total	C	N	O	0	0
			11	6	1	4		
5	O	1	Total	C	N	O	0	0
			11	6	1	4		
5	P	1	Total	C	N	O	0	0
			11	6	1	4		
5	Q	1	Total	C	N	O	0	0
			11	6	1	4		
5	R	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	M	155	Total	O	0	0
			155	155		
6	B	78	Total	O	0	0
			78	78		
6	N	163	Total	O	0	0
			163	163		

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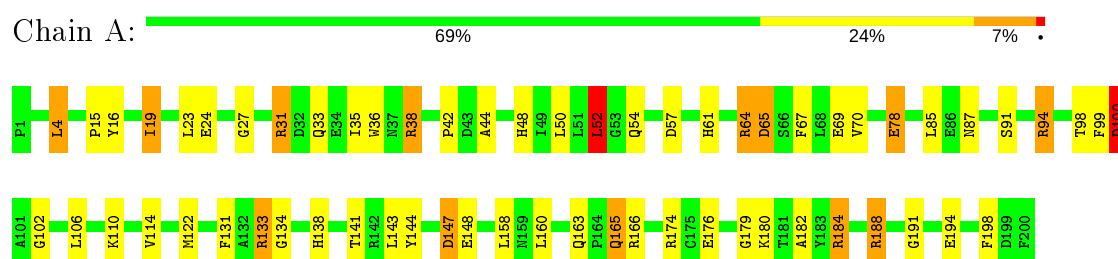
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	76	Total 76	O 76	0	0
6	O	158	Total 158	O 158	0	0
6	D	79	Total 79	O 79	0	0
6	P	149	Total 149	O 149	0	0
6	E	81	Total 81	O 81	0	0
6	Q	160	Total 160	O 160	0	0
6	F	75	Total 75	O 75	0	0
6	R	163	Total 163	O 163	0	0

3 Residue-property plots

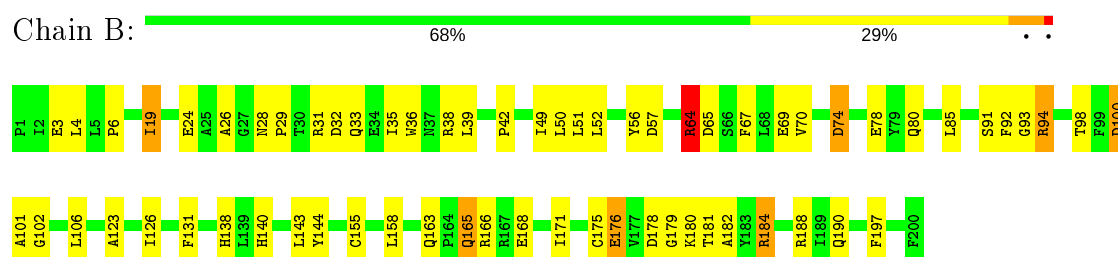
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

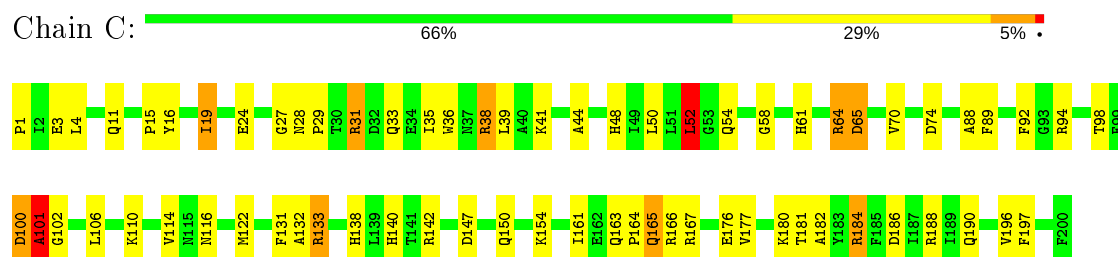
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



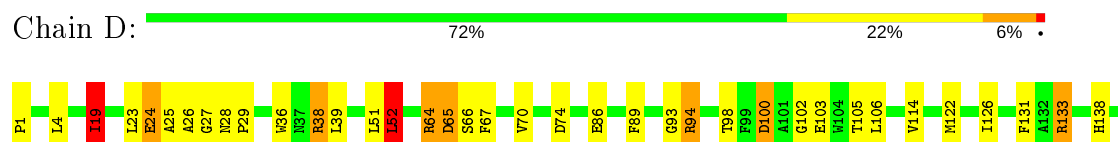
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

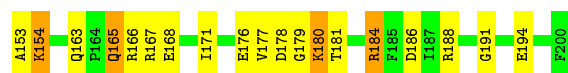


• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



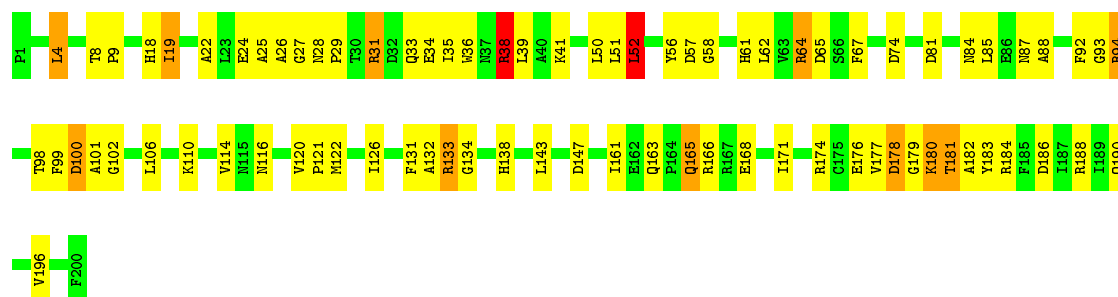
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





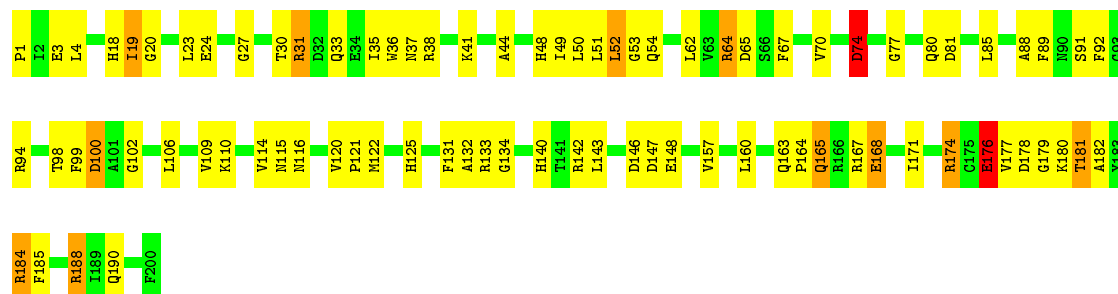
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 60% 34% 6%



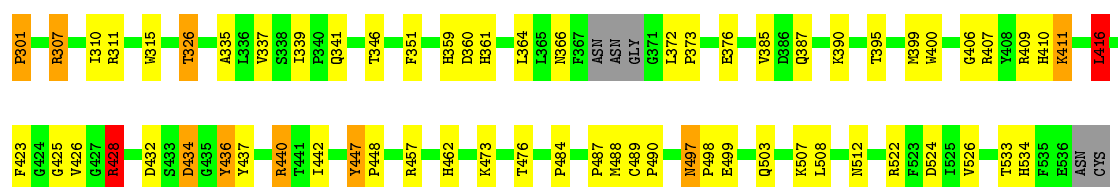
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 58% 36% 6%



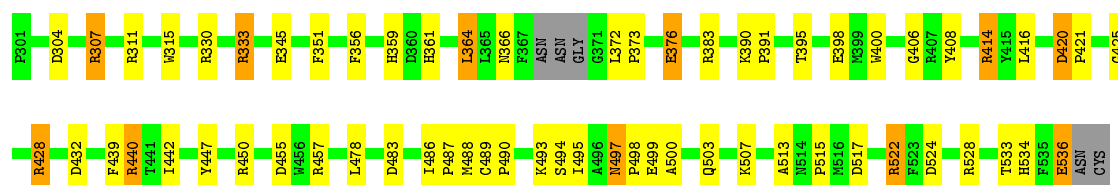
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 71% 23% 6%

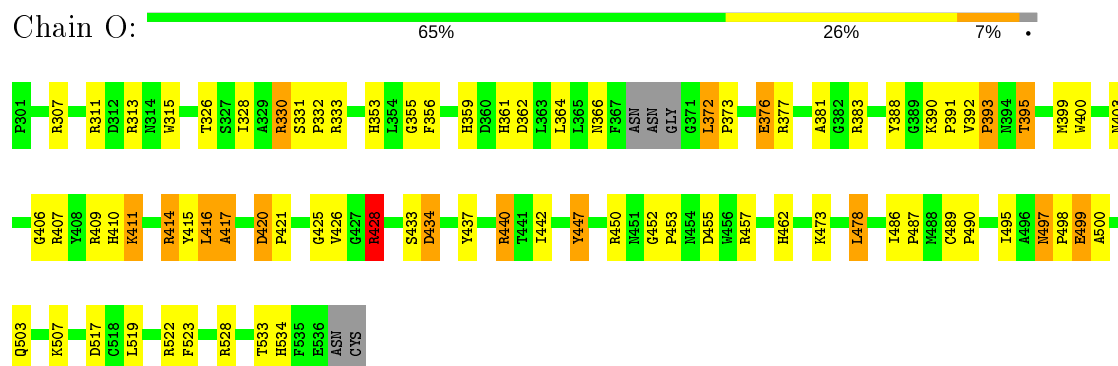


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

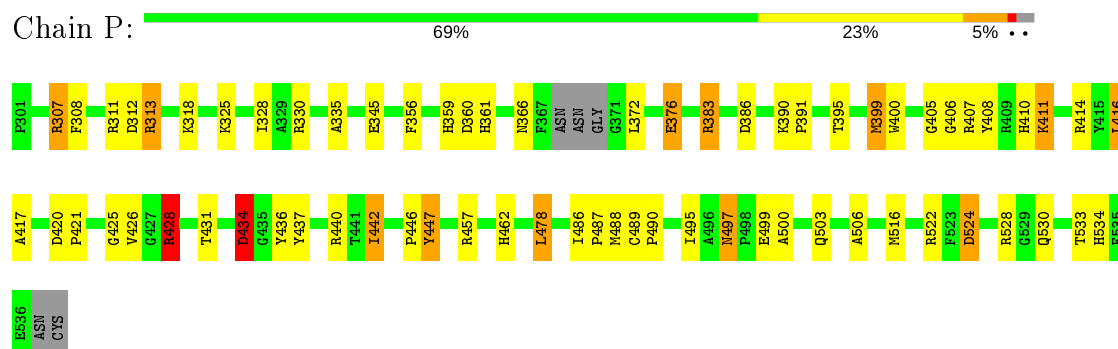
Chain N: 71% 22% 5%



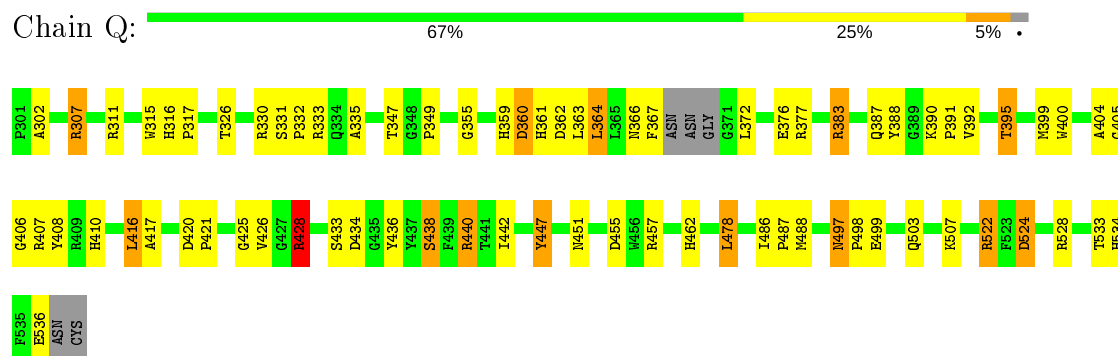
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

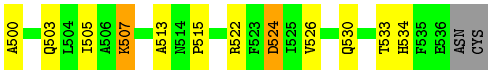


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





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	196.20 Å 127.10 Å 133.70 Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.13	Depositor
% Data completeness (in resolution range)	96.0 (6.00-2.13)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21978	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: INO, FE, BME

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	1.00	2/1611 (0.1%)	1.73	30/2195 (1.4%)
1	B	0.99	0/1611	1.73	29/2195 (1.3%)
1	C	0.99	0/1611	1.59	20/2195 (0.9%)
1	D	1.01	0/1611	1.65	29/2195 (1.3%)
1	E	1.02	0/1611	1.63	21/2195 (1.0%)
1	F	1.08	1/1611 (0.1%)	1.69	28/2195 (1.3%)
2	M	1.04	0/1895	1.65	20/2580 (0.8%)
2	N	1.05	2/1895 (0.1%)	1.66	32/2580 (1.2%)
2	O	1.04	0/1895	1.66	34/2580 (1.3%)
2	P	1.05	1/1895 (0.1%)	1.61	27/2580 (1.0%)
2	Q	1.07	2/1895 (0.1%)	1.60	20/2580 (0.8%)
2	R	1.08	1/1895 (0.1%)	1.64	33/2580 (1.3%)
All	All	1.04	9/21036 (0.0%)	1.65	323/28650 (1.1%)

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	B	0	1
2	R	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-6.43	1.35	1.46
2	Q	367	PHE	C-O	5.66	1.34	1.23
2	P	345	GLU	CD-OE1	-5.37	1.19	1.25
2	N	398	GLU	CD-OE1	-5.17	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	433	SER	CB-OG	5.14	1.49	1.42
2	R	398	GLU	CD-OE1	-5.07	1.20	1.25
2	N	345	GLU	CD-OE1	-5.02	1.20	1.25
1	F	133	ARG	CD-NE	-5.01	1.38	1.46
1	A	94	ARG	CG-CD	-5.00	1.39	1.51

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	440	ARG	NE-CZ-NH2	-23.91	108.35	120.30
2	R	440	ARG	NE-CZ-NH2	-22.66	108.97	120.30
2	M	440	ARG	NE-CZ-NH2	-22.31	109.14	120.30
2	P	440	ARG	NE-CZ-NH2	-20.43	110.09	120.30
2	O	440	ARG	NE-CZ-NH2	-19.72	110.44	120.30
1	F	133	ARG	CD-NE-CZ	18.14	148.99	123.60
2	Q	440	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	A	166	ARG	NE-CZ-NH1	16.25	128.42	120.30
1	B	184	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	A	94	ARG	CD-NE-CZ	15.35	145.09	123.60
1	F	133	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	B	166	ARG	NE-CZ-NH1	14.53	127.56	120.30
1	D	94	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	A	94	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	B	64	ARG	NE-CZ-NH1	-13.88	113.36	120.30
1	C	188	ARG	NE-CZ-NH1	13.54	127.07	120.30
2	O	313	ARG	NE-CZ-NH1	13.49	127.05	120.30
1	E	94	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	A	64	ARG	NE-CZ-NH1	-12.91	113.84	120.30
2	Q	428	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	F	64	ARG	NE-CZ-NH1	-12.72	113.94	120.30
2	O	528	ARG	NE-CZ-NH2	-12.43	114.09	120.30
2	N	457	ARG	NE-CZ-NH2	-12.42	114.09	120.30
2	Q	457	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	D	167	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	B	166	ARG	NE-CZ-NH2	-12.33	114.13	120.30
1	D	166	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	E	64	ARG	NE-CZ-NH1	-11.68	114.46	120.30
2	O	333	ARG	NE-CZ-NH2	-11.62	114.49	120.30
2	N	440	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	B	188	ARG	NE-CZ-NH2	-11.51	114.55	120.30
2	R	428	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	E	166	ARG	NE-CZ-NH1	11.16	125.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	188	ARG	NE-CZ-NH1	11.00	125.80	120.30
2	P	457	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	A	133	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	D	133	ARG	NE-CZ-NH1	10.73	125.66	120.30
2	Q	377	ARG	NE-CZ-NH1	-10.71	114.94	120.30
1	F	38	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	D	64	ARG	NE-CZ-NH1	-10.50	115.05	120.30
2	Q	457	ARG	NE-CZ-NH2	-10.33	115.13	120.30
2	M	457	ARG	CD-NE-CZ	10.29	138.00	123.60
1	B	38	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	E	94	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	B	94	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	C	133	ARG	NE-CZ-NH1	9.93	125.27	120.30
2	M	440	ARG	NE-CZ-NH1	9.92	125.26	120.30
2	P	524	ASP	CB-CG-OD1	9.91	127.22	118.30
2	O	457	ARG	NE-CZ-NH1	9.87	125.23	120.30
2	R	307	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	O	457	ARG	NE-CZ-NH2	-9.77	115.41	120.30
2	R	383	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	D	94	ARG	NE-CZ-NH1	9.60	125.10	120.30
2	P	457	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	94	ARG	CG-CD-NE	9.37	131.48	111.80
2	M	524	ASP	CB-CG-OD1	9.33	126.69	118.30
2	O	517	ASP	CB-CG-OD1	9.30	126.67	118.30
2	P	440	ARG	NE-CZ-NH1	9.20	124.90	120.30
2	Q	333	ARG	NE-CZ-NH2	-9.19	115.70	120.30
1	A	166	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	E	38	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	N	333	ARG	NE-CZ-NH2	-9.09	115.76	120.30
2	Q	440	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	D	188	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	M	307	ARG	NE-CZ-NH1	8.96	124.78	120.30
2	N	428	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	166	ARG	CD-NE-CZ	8.86	136.00	123.60
2	N	522	ARG	CD-NE-CZ	8.83	135.97	123.60
1	F	38	ARG	NE-CZ-NH2	-8.73	115.94	120.30
2	O	457	ARG	CD-NE-CZ	8.71	135.79	123.60
1	D	167	ARG	CD-NE-CZ	8.66	135.73	123.60
1	B	64	ARG	CD-NE-CZ	-8.61	111.54	123.60
1	B	184	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	E	166	ARG	NE-CZ-NH2	-8.59	116.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	407	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	Q	524	ASP	CB-CG-OD1	8.51	125.96	118.30
1	F	64	ARG	CD-NE-CZ	-8.34	111.92	123.60
1	C	133	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	F	31	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	186	ASP	CB-CG-OD1	8.23	125.71	118.30
2	O	517	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	D	133	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	31	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	P	313	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	P	307	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	166	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	94	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	Q	524	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	D	188	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	C	52	LEU	CB-CA-C	7.94	125.29	110.20
2	M	457	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	E	31	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	D	186	ASP	CB-CG-OD2	-7.84	111.24	118.30
2	M	428	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	F	142	ARG	NE-CZ-NH2	-7.82	116.39	120.30
2	N	414	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	E	186	ASP	CB-CG-OD1	7.77	125.29	118.30
2	R	428	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	N	524	ASP	CB-CG-OD2	-7.76	111.31	118.30
2	R	432	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	D	167	ARG	NE-CZ-NH2	-7.73	116.43	120.30
2	M	407	ARG	NE-CZ-NH1	7.71	124.15	120.30
2	O	409	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	D	166	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	64	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	F	146	ASP	CB-CG-OD1	7.60	125.14	118.30
2	P	478	LEU	CA-CB-CG	7.54	132.65	115.30
1	B	94	ARG	CG-CD-NE	7.50	127.55	111.80
2	R	311	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	C	65	ASP	CB-CG-OD1	7.47	125.02	118.30
1	F	174	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	Q	383	ARG	CD-NE-CZ	-7.39	113.25	123.60
1	A	31	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	N	420	ASP	CB-CG-OD2	-7.37	111.67	118.30
2	P	447	TYR	CB-CG-CD2	7.35	125.41	121.00
1	E	133	ARG	NE-CZ-NH2	-7.30	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CB-CG-CD	7.29	130.56	111.60
1	A	133	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	N	383	ARG	CD-NE-CZ	-7.26	113.44	123.60
1	A	64	ARG	CD-NE-CZ	-7.25	113.46	123.60
2	O	353	HIS	CA-CB-CG	-7.21	101.34	113.60
1	C	38	ARG	CD-NE-CZ	-7.21	113.51	123.60
2	P	428	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	184	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	52	LEU	CA-CB-CG	7.15	131.75	115.30
1	F	142	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	31	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	R	414	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	64	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	N	450	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	E	81	ASP	CB-CG-OD1	7.01	124.61	118.30
2	N	457	ARG	NE-CZ-NH1	7.01	123.80	120.30
2	M	436	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	M	311	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	N	307	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	65	ASP	CB-CG-OD1	6.92	124.53	118.30
2	O	420	ASP	CB-CG-OD1	6.91	124.52	118.30
2	R	440	ARG	NH1-CZ-NH2	6.88	126.96	119.40
1	A	23	LEU	CB-CA-C	6.87	123.25	110.20
2	N	524	ASP	CB-CG-OD1	6.85	124.46	118.30
2	N	311	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	O	434	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	O	440	ARG	NH1-CZ-NH2	6.80	126.88	119.40
1	E	64	ARG	CD-NE-CZ	-6.80	114.08	123.60
1	A	52	LEU	CB-CA-C	6.77	123.07	110.20
1	C	31	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	E	133	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	M	428	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	F	74	ASP	CB-CG-OD1	6.71	124.34	118.30
2	P	386	ASP	CB-CG-OD2	6.70	124.33	118.30
2	R	376	GLU	OE1-CD-OE2	6.68	131.32	123.30
2	R	434	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	F	64	ARG	NE-CZ-NH2	6.61	123.61	120.30
2	O	377	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	101	ALA	CB-CA-C	-6.58	100.24	110.10
1	D	65	ASP	CB-CG-OD1	6.57	124.21	118.30
2	O	377	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	166	ARG	CD-NE-CZ	6.49	132.68	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	457	ARG	CD-NE-CZ	6.46	132.65	123.60
1	D	86	GLU	CG-CD-OE1	6.46	131.21	118.30
1	E	38	ARG	CD-NE-CZ	-6.43	114.59	123.60
2	R	330	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	101	ALA	N-CA-CB	-6.41	101.12	110.10
1	C	184	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	P	524	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	F	133	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	M	428	ARG	CD-NE-CZ	6.33	132.47	123.60
2	Q	434	ASP	CB-CG-OD2	-6.33	112.61	118.30
2	Q	307	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	R	457	ARG	CA-CB-CG	6.31	127.28	113.40
2	N	528	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	F	167	ARG	CD-NE-CZ	-6.31	114.77	123.60
2	M	447	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	E	74	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	36	TRP	CB-CA-C	6.25	122.91	110.40
1	A	100	ASP	CB-CG-OD2	6.24	123.91	118.30
2	P	312	ASP	CB-CG-OD1	6.20	123.88	118.30
1	F	176	GLU	CG-CD-OE1	6.20	130.70	118.30
2	Q	360	ASP	CB-CG-OD1	6.19	123.87	118.30
2	N	517	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	94	ARG	CB-CG-CD	6.18	127.67	111.60
2	R	524	ASP	CB-CG-OD1	6.16	123.85	118.30
2	N	311	ARG	CD-NE-CZ	6.16	132.22	123.60
1	F	184	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	E	38	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	R	361	HIS	CA-CB-CG	-6.14	103.16	113.60
1	A	188	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	Q	360	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	P	428	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	O	428	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	F	52	LEU	CA-CB-CG	6.08	129.28	115.30
1	B	78	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	F	62	LEU	CA-CB-CG	6.05	129.22	115.30
1	C	36	TRP	CB-CA-C	6.04	122.48	110.40
1	B	31	ARG	CD-NE-CZ	6.03	132.04	123.60
2	R	450	ARG	CD-NE-CZ	-5.99	115.21	123.60
2	M	447	TYR	N-CA-CB	-5.99	99.82	110.60
1	A	174	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	65	ASP	CB-CG-OD1	5.97	123.67	118.30
2	M	447	TYR	CB-CG-CD2	5.96	124.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	376	GLU	CG-CD-OE2	-5.95	106.40	118.30
2	P	528	ARG	CD-NE-CZ	5.94	131.92	123.60
2	N	383	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	57	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	Q	522	ARG	NE-CZ-NH1	-5.89	117.36	120.30
2	M	409	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	E	52	LEU	CB-CA-C	5.87	121.36	110.20
2	P	447	TYR	CB-CG-CD1	-5.86	117.48	121.00
2	N	450	ARG	CD-NE-CZ	5.86	131.80	123.60
2	N	483	ASP	CB-CG-OD2	5.83	123.55	118.30
2	N	376	GLU	OE1-CD-OE2	5.82	130.29	123.30
2	O	388	TYR	CB-CG-CD1	-5.82	117.51	121.00
2	O	499	GLU	CG-CD-OE1	5.80	129.90	118.30
2	Q	330	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	142	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	D	19	ILE	CB-CA-C	5.79	123.17	111.60
2	M	416	LEU	CA-CB-CG	5.78	128.59	115.30
1	C	94	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	D	38	ARG	CD-NE-CZ	-5.76	115.53	123.60
1	F	140	HIS	CB-CA-C	-5.76	98.88	110.40
1	E	36	TRP	CB-CA-C	5.75	121.91	110.40
2	O	447	TYR	N-CA-CB	-5.74	100.27	110.60
1	E	57	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	147	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	P	330	ARG	CD-NE-CZ	-5.73	115.58	123.60
1	D	24	GLU	CA-CB-CG	5.71	125.97	113.40
2	N	383	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	O	313	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	N	304	ASP	CB-CG-OD1	5.67	123.41	118.30
1	F	52	LEU	CB-CA-C	5.66	120.95	110.20
2	N	455	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	64	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	P	414	ARG	CD-NE-CZ	-5.63	115.72	123.60
1	D	64	ARG	CD-NE-CZ	-5.62	115.73	123.60
1	F	65	ASP	CB-CG-OD1	5.62	123.35	118.30
2	O	311	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	E	81	ASP	CB-CG-OD2	-5.60	113.26	118.30
2	P	447	TYR	N-CA-CB	-5.60	100.53	110.60
2	N	440	ARG	NH1-CZ-NH2	5.58	125.54	119.40
2	R	353	HIS	CA-CB-CG	-5.57	104.13	113.60
1	D	52	LEU	CB-CA-C	5.54	120.73	110.20
2	R	440	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	383	ARG	NE-CZ-NH1	-5.53	117.53	120.30
2	R	499	GLU	N-CA-CB	5.53	120.56	110.60
1	D	186	ASP	CB-CG-OD1	5.52	123.27	118.30
2	O	428	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	E	52	LEU	CA-CB-CG	5.51	127.97	115.30
2	Q	447	TYR	CB-CG-CD2	5.51	124.31	121.00
2	O	417	ALA	CB-CA-C	5.50	118.35	110.10
1	B	175	CYS	CA-CB-SG	5.47	123.86	114.00
2	O	452	GLY	N-CA-C	-5.44	99.49	113.10
2	P	506	ALA	CB-CA-C	5.44	118.26	110.10
2	R	455	ASP	CB-CG-OD1	5.43	123.19	118.30
2	R	312	ASP	CB-CG-OD1	-5.42	113.42	118.30
2	O	455	ASP	CB-CG-OD1	5.42	123.17	118.30
2	P	376	GLU	CG-CD-OE2	-5.41	107.47	118.30
2	O	409	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	D	94	ARG	CG-CD-NE	5.39	123.11	111.80
2	R	313	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	R	407	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	N	414	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	F	38	ARG	CA-CB-CG	5.35	125.17	113.40
2	O	383	ARG	N-CA-CB	-5.34	100.98	110.60
1	B	176	GLU	CB-CG-CD	5.34	128.61	114.20
2	P	428	ARG	CG-CD-NE	5.33	123.00	111.80
1	A	38	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	141	THR	CA-CB-CG2	5.31	119.83	112.40
2	O	450	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	Q	330	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	57	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	N	330	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	103	GLU	CG-CD-OE1	-5.29	107.71	118.30
1	B	36	TRP	CB-CA-C	5.28	120.96	110.40
1	D	74	ASP	CB-CG-OD1	5.27	123.05	118.30
2	N	432	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	178	ASP	CB-CG-OD2	5.25	123.02	118.30
1	F	31	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	R	499	GLU	CA-CB-CG	5.24	124.92	113.40
1	D	184	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	Q	311	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	P	383	ARG	CD-NE-CZ	-5.23	116.28	123.60
1	B	56	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	87	ASN	CA-CB-CG	5.22	124.88	113.40
2	R	372	LEU	N-CA-CB	-5.20	99.99	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	GLN	N-CA-CB	5.20	119.95	110.60
1	B	24	GLU	CG-CD-OE2	5.19	128.69	118.30
1	B	31	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	P	434	ASP	CB-CG-OD1	-5.19	113.63	118.30
2	Q	528	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	11	GLN	N-CA-CB	5.16	119.89	110.60
2	O	376	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	D	23	LEU	CB-CA-C	5.13	119.95	110.20
2	R	452	GLY	N-CA-C	-5.12	100.29	113.10
1	A	36	TRP	CB-CA-C	5.12	120.65	110.40
2	P	434	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	94	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	F	168	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	B	74	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	94	ARG	CG-CD-NE	5.10	122.50	111.80
2	P	440	ARG	NH1-CZ-NH2	5.09	125.00	119.40
2	N	536	GLU	CG-CD-OE1	5.08	128.47	118.30
1	F	74	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	66	SER	N-CA-CB	5.07	118.11	110.50
2	P	311	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	N	439	PHE	O-C-N	5.07	130.81	122.70
1	C	64	ARG	CD-NE-CZ	-5.07	116.51	123.60
2	O	414	ARG	CD-NE-CZ	-5.06	116.51	123.60
2	R	434	ASP	OD1-CG-OD2	5.06	132.91	123.30
1	D	133	ARG	CD-NE-CZ	5.06	130.68	123.60
2	O	383	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	184	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	F	36	TRP	CB-CA-C	5.04	120.47	110.40
2	R	434	ASP	CA-CB-CG	-5.03	102.33	113.40
2	M	476	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	78	GLU	OE1-CD-OE2	5.03	129.33	123.30
2	R	428	ARG	CG-CD-NE	5.02	122.35	111.80
2	M	409	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	M	432	ASP	CB-CG-OD1	5.01	122.81	118.30
2	R	345	GLU	CG-CD-OE2	-5.01	108.28	118.30
2	R	457	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	O	330	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	F	188	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	ARG	Sidechain
2	R	407	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	57	0
1	B	1571	0	1499	48	0
1	C	1571	0	1499	56	0
1	D	1571	0	1499	42	0
1	E	1571	0	1499	71	0
1	F	1571	0	1499	77	0
2	M	1840	0	1793	58	0
2	N	1840	0	1793	44	0
2	O	1840	0	1793	56	0
2	P	1840	0	1793	47	0
2	Q	1840	0	1793	60	0
2	R	1840	0	1793	68	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	4	0	5	0	0
4	N	4	0	5	1	0
4	O	4	0	5	0	0
4	P	4	0	5	0	0
4	Q	4	0	5	1	0
4	R	4	0	5	0	0
5	M	11	0	3	0	0
5	N	11	0	3	0	0
5	O	11	0	3	0	0
5	P	11	0	3	0	0
5	Q	11	0	3	0	0
5	R	11	0	3	1	0
6	A	79	0	0	1	0
6	B	78	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	76	0	0	2	0
6	D	79	0	0	0	0
6	E	81	0	0	0	0
6	F	75	0	0	1	0
6	M	155	0	0	3	0
6	N	163	0	0	6	0
6	O	158	0	0	7	0
6	P	149	0	0	3	0
6	Q	160	0	0	6	0
6	R	163	0	0	4	0
All	All	21978	0	19800	607	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 15.

All (607) 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:B:165:GLN:NE2	1:B:165:GLN:H	1.34	1.26
1:E:165:GLN:NE2	1:E:165:GLN:H	1.36	1.22
1:E:165:GLN:N	1:E:165:GLN:HE21	1.40	1.18
2:R:497:ASN:ND2	2:R:499:GLU:H	1.48	1.12
1:A:134:GLY:CA	2:M:326:THR:HG22	1.88	1.04
1:B:165:GLN:N	1:B:165:GLN:HE21	1.60	0.97
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.54	0.89
2:R:361:HIS:H	2:R:361:HIS:CD2	1.90	0.89
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.73	0.89
1:B:165:GLN:HE21	1:B:165:GLN:H	0.96	0.89
1:B:165:GLN:N	1:B:165:GLN:NE2	2.18	0.88
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.39	0.87
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.90	0.86
2:M:497:ASN:ND2	2:M:499:GLU:H	1.73	0.85
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.40	0.85
2:R:497:ASN:HD22	2:R:497:ASN:C	1.83	0.82
2:R:497:ASN:ND2	2:R:499:GLU:N	2.28	0.82
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.15	0.81
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.62	0.81
2:R:497:ASN:HD22	2:R:498:PRO:N	1.77	0.81
2:M:390:LYS:HD2	6:M:643:HOH:O	1.80	0.80
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.13	0.80
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:390:LYS:HD3	6:Q:670:HOH:O	1.81	0.80
2:R:497:ASN:HD22	2:R:499:GLU:H	1.30	0.79
2:R:361:HIS:H	2:R:361:HIS:HD2	1.29	0.79
2:N:497:ASN:ND2	2:N:499:GLU:HB2	1.97	0.79
1:E:19:ILE:HD11	2:Q:408:TYR:HD1	1.47	0.79
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.63	0.79
1:F:165:GLN:NE2	1:F:165:GLN:H	1.80	0.79
2:P:390:LYS:HD2	6:P:683:HOH:O	1.82	0.78
2:Q:390:LYS:HE2	6:Q:747:HOH:O	1.83	0.78
2:R:497:ASN:HD21	2:R:499:GLU:H	1.32	0.78
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.82	0.76
2:N:497:ASN:HD22	2:N:499:GLU:H	1.31	0.76
1:A:176:GLU:HG3	1:A:180:LYS:O	1.87	0.75
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.16	0.75
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.04	0.75
1:A:134:GLY:HA2	2:M:326:THR:HG22	1.68	0.74
2:Q:522:ARG:NH1	6:Q:691:HOH:O	2.20	0.74
2:M:361:HIS:H	2:M:361:HIS:CD2	2.04	0.74
1:D:180:LYS:HG3	1:D:181:THR:N	2.03	0.73
1:E:98:THR:O	1:E:102:GLY:HA2	1.89	0.73
1:D:19:ILE:HD11	2:P:408:TYR:HD2	1.53	0.73
1:D:165:GLN:H	1:D:165:GLN:NE2	1.86	0.73
2:Q:497:ASN:HD22	2:Q:497:ASN:C	1.92	0.73
2:N:489:CYS:O	2:N:493:LYS:HG3	1.89	0.72
2:P:497:ASN:HD22	2:P:499:GLU:H	1.38	0.72
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.54	0.71
2:M:310:ILE:HD12	2:O:453:PRO:HB2	1.72	0.71
1:B:176:GLU:HG3	1:B:180:LYS:C	2.11	0.71
1:C:165:GLN:NE2	1:C:165:GLN:H	1.88	0.71
2:M:497:ASN:HD22	2:M:499:GLU:H	1.37	0.71
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.35	0.71
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.25	0.71
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.91	0.71
2:P:361:HIS:CD2	2:P:361:HIS:H	2.07	0.71
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.56	0.70
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.07	0.70
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.72	0.70
1:E:180:LYS:HG3	1:E:181:THR:N	2.05	0.70
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.74	0.69
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.73	0.69
1:B:176:GLU:HG3	1:B:180:LYS:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PHE:O	1:C:132:ALA:HB2	1.92	0.69
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.07	0.69
2:N:359:HIS:O	2:N:366:ASN:HB3	1.92	0.69
1:F:163:GLN:HB3	1:F:165:GLN:HE21	1.58	0.69
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.58	0.68
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.08	0.68
2:N:494:SER:O	6:N:780:HOH:O	2.11	0.68
1:F:70:VAL:HG21	1:F:106:LEU:HD21	1.74	0.68
2:N:361:HIS:H	2:N:361:HIS:CD2	2.11	0.68
1:E:110:LYS:NZ	1:E:183:TYR:OH	2.27	0.68
1:C:44:ALA:O	1:C:48:HIS:NE2	2.21	0.68
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.76	0.67
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.15	0.67
2:O:416:LEU:C	2:O:416:LEU:HD23	2.14	0.67
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.30	0.66
2:O:522:ARG:NH1	6:O:716:HOH:O	2.18	0.66
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.77	0.66
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.78	0.66
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.44	0.66
1:E:19:ILE:O	2:Q:426:VAL:HG21	1.95	0.66
1:C:65:ASP:OD2	1:C:133:ARG:HD3	1.96	0.66
1:F:188:ARG:HH11	1:F:188:ARG:HG3	1.59	0.66
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.63	0.66
1:C:176:GLU:HG3	1:C:180:LYS:O	1.96	0.66
2:M:361:HIS:HD2	2:M:361:HIS:H	1.43	0.66
1:C:16:TYR:O	1:C:19:ILE:HG23	1.96	0.65
2:N:406:GLY:O	2:N:447:TYR:HD2	1.79	0.65
2:Q:388:TYR:OH	6:Q:621:HOH:O	2.13	0.65
1:B:98:THR:O	1:B:102:GLY:HA2	1.97	0.65
1:C:177:VAL:O	1:C:180:LYS:HB3	1.97	0.65
1:E:39:LEU:CD1	1:E:106:LEU:HD11	2.27	0.65
1:F:147:ASP:OD2	1:F:174:ARG:HD2	1.97	0.65
1:E:19:ILE:HG21	2:Q:410:HIS:HB2	1.78	0.65
1:C:110:LYS:NZ	1:C:147:ASP:OD1	2.30	0.64
2:O:361:HIS:CD2	2:O:361:HIS:H	2.12	0.64
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.78	0.64
1:C:52:LEU:HD22	1:C:52:LEU:C	2.17	0.64
1:A:134:GLY:HA3	2:M:326:THR:CG2	2.27	0.64
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.80	0.64
2:R:415:TYR:CE1	2:R:416:LEU:CD2	2.81	0.64
1:F:177:VAL:HG12	1:F:178:ASP:OD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PRO:HB2	2:N:503:GLN:HE22	1.63	0.63
2:R:522:ARG:NH1	6:R:812:HOH:O	2.32	0.63
1:F:98:THR:OG1	1:F:102:GLY:N	2.32	0.63
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.12	0.63
1:E:19:ILE:HD11	2:Q:408:TYR:CD1	2.33	0.63
1:A:133:ARG:HG3	2:M:326:THR:HG21	1.81	0.63
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.80	0.62
2:P:416:LEU:HD23	2:P:416:LEU:C	2.20	0.62
2:N:400:TRP:HA	2:N:425:GLY:O	1.99	0.62
2:O:390:LYS:HE2	6:O:798:HOH:O	1.99	0.62
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.99	0.62
1:F:50:LEU:O	1:F:182:ALA:HA	2.00	0.62
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.63	0.62
2:R:473:LYS:NZ	6:R:859:HOH:O	2.32	0.62
1:C:180:LYS:HD2	1:C:181:THR:H	1.65	0.61
1:F:48:HIS:C	1:F:180:LYS:NZ	2.53	0.61
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.34	0.61
2:R:361:HIS:N	2:R:361:HIS:CD2	2.62	0.61
1:F:177:VAL:O	1:F:180:LYS:HB3	2.00	0.61
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.48	0.61
2:N:497:ASN:ND2	2:N:499:GLU:H	1.99	0.61
2:P:383:ARG:NH2	2:P:391:PRO:HG3	2.14	0.61
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.82	0.61
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.65	0.61
1:A:165:GLN:H	1:A:165:GLN:CD	2.04	0.61
1:F:64:ARG:NE	1:F:100:ASP:O	2.30	0.61
1:F:180:LYS:HD2	1:F:181:THR:N	2.16	0.61
1:A:78:GLU:CG	2:M:301:PRO:HG3	2.29	0.61
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	1.99	0.61
1:A:19:ILE:O	2:M:426:VAL:HG21	2.01	0.60
1:C:180:LYS:HD2	1:C:181:THR:N	2.16	0.60
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.49	0.60
2:R:400:TRP:HA	2:R:425:GLY:O	2.02	0.60
1:C:100:ASP:OD1	1:C:100:ASP:N	2.35	0.60
1:F:77:GLY:O	1:F:114:VAL:HG12	2.02	0.60
2:N:361:HIS:HD2	2:N:361:HIS:H	1.49	0.60
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.83	0.60
2:M:522:ARG:NH1	6:M:664:HOH:O	2.29	0.60
2:M:497:ASN:HD22	2:M:498:PRO:N	2.00	0.59
2:O:359:HIS:O	2:O:366:ASN:HB3	2.02	0.59
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.38	0.59
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.01	0.59
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.38	0.59
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.17	0.59
2:Q:405:GLY:HA3	6:Q:673:HOH:O	2.03	0.59
1:A:134:GLY:CA	2:M:326:THR:CG2	2.76	0.58
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.38	0.58
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.51	0.58
2:R:406:GLY:O	2:R:447:TYR:HD1	1.86	0.58
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.36	0.58
2:P:361:HIS:HD2	2:P:361:HIS:H	1.49	0.58
2:O:497:ASN:ND2	2:O:499:GLU:H	2.02	0.58
1:D:24:GLU:O	1:D:27:GLY:N	2.33	0.58
2:N:390:LYS:CD	6:N:743:HOH:O	2.52	0.58
2:P:416:LEU:HD23	2:P:417:ALA:N	2.19	0.58
1:F:176:GLU:HG3	1:F:180:LYS:N	2.18	0.58
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.39	0.57
1:F:44:ALA:O	1:F:48:HIS:NE2	2.32	0.57
2:O:406:GLY:O	2:O:447:TYR:HD1	1.87	0.57
2:P:497:ASN:ND2	2:P:499:GLU:H	2.02	0.57
1:A:176:GLU:HA	1:A:180:LYS:O	2.05	0.57
1:A:98:THR:O	1:A:102:GLY:HA2	2.04	0.57
1:D:19:ILE:HG22	1:D:26:ALA:HB1	1.85	0.57
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.85	0.57
1:D:19:ILE:O	2:P:426:VAL:HG21	2.04	0.57
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.03	0.57
1:E:24:GLU:O	1:E:27:GLY:N	2.35	0.57
1:F:74:ASP:HB2	6:F:690:HOH:O	2.04	0.57
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.35	0.57
1:E:56:TYR:CE1	1:E:62:LEU:HD23	2.39	0.57
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.01	0.57
1:D:64:ARG:NE	1:D:100:ASP:O	2.37	0.57
2:M:473:LYS:NZ	6:M:651:HOH:O	2.38	0.57
1:D:19:ILE:HG21	2:P:410:HIS:HB2	1.87	0.57
1:D:177:VAL:O	1:D:180:LYS:HB3	2.05	0.57
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.23	0.57
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.05	0.57
1:F:74:ASP:HB3	1:F:89:PHE:CE2	2.40	0.57
1:E:64:ARG:NE	1:E:100:ASP:O	2.31	0.56
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.02	0.56
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:O	1:D:105:THR:HA	2.05	0.56
1:F:48:HIS:O	1:F:180:LYS:NZ	2.38	0.56
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.87	0.56
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.21	0.56
2:M:399:MET:HA	2:M:462:HIS:O	2.06	0.56
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.40	0.56
1:F:176:GLU:HG3	1:F:180:LYS:O	2.05	0.56
1:F:157:VAL:O	1:F:160:LEU:HB2	2.06	0.55
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.88	0.55
2:Q:536:GLU:HB2	6:Q:723:HOH:O	2.05	0.55
2:R:313:ARG:O	2:R:318:LYS:HD3	2.07	0.55
1:F:110:LYS:NZ	1:F:147:ASP:OD1	2.39	0.55
2:N:486:ILE:HB	2:N:487:PRO:HD3	1.88	0.55
2:R:497:ASN:ND2	2:R:497:ASN:C	2.55	0.55
2:O:376:GLU:O	2:O:442:ILE:HA	2.07	0.55
1:F:54:GLN:HG3	1:F:184:ARG:HH22	1.72	0.55
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.87	0.55
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.70	0.55
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.88	0.55
1:F:50:LEU:HD12	1:F:51:LEU:N	2.22	0.55
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.89	0.55
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.89	0.55
1:A:78:GLU:HG2	2:M:301:PRO:HB2	1.88	0.55
2:R:314:ASN:OD1	2:R:318:LYS:HE2	2.07	0.54
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.41	0.54
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.88	0.54
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.71	0.54
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.90	0.54
1:E:39:LEU:HD13	1:E:106:LEU:HD11	1.88	0.54
1:A:69:GLU:OE1	2:M:473:LYS:HE2	2.07	0.54
2:R:405:GLY:HA3	6:R:791:HOH:O	2.07	0.54
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.07	0.54
1:F:165:GLN:CD	1:F:165:GLN:H	2.11	0.54
2:O:361:HIS:HD2	6:O:766:HOH:O	1.89	0.54
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.08	0.54
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.23	0.54
2:R:478:LEU:C	2:R:478:LEU:HD23	2.28	0.54
2:N:497:ASN:HD22	2:N:499:GLU:N	2.03	0.54
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.75	0.54
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.73	0.54
2:M:448:PRO:HB2	2:P:516:MET:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:ILE:CG2	2:Q:410:HIS:HB2	2.37	0.54
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.91	0.53
1:F:54:GLN:HG3	1:F:184:ARG:NH2	2.23	0.53
2:N:478:LEU:HD23	2:N:478:LEU:C	2.29	0.53
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.44	0.53
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.42	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.09	0.53
1:B:176:GLU:HG2	1:B:180:LYS:N	2.23	0.53
1:E:92:PHE:CD1	2:Q:349:PRO:HG3	2.43	0.53
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.90	0.53
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.91	0.53
1:C:19:ILE:O	2:O:426:VAL:HG21	2.08	0.53
1:F:98:THR:O	1:F:102:GLY:HA2	2.08	0.53
2:R:399:MET:HA	2:R:462:HIS:O	2.09	0.53
1:A:100:ASP:N	1:A:100:ASP:OD1	2.41	0.53
1:F:114:VAL:HG23	1:F:122:MET:CE	2.39	0.53
1:F:110:LYS:NZ	1:F:148:GLU:OE2	2.40	0.53
2:O:400:TRP:HA	2:O:425:GLY:O	2.09	0.53
2:O:307:ARG:HG2	2:O:533:THR:HG22	1.89	0.53
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.41	0.53
1:F:100:ASP:N	1:F:100:ASP:OD1	2.41	0.53
2:R:497:ASN:HD22	2:R:499:GLU:N	1.96	0.53
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.07	0.52
2:O:399:MET:HA	2:O:462:HIS:O	2.09	0.52
1:F:131:PHE:O	1:F:132:ALA:HB2	2.09	0.52
2:O:407:ARG:NH1	2:O:417:ALA:O	2.37	0.52
2:P:406:GLY:O	2:P:447:TYR:HD1	1.92	0.52
1:D:114:VAL:HG23	1:D:122:MET:CE	2.40	0.52
1:E:177:VAL:HG12	1:E:178:ASP:OD2	2.09	0.52
2:R:487:PRO:O	2:R:493:LYS:HD3	2.09	0.52
2:P:431:THR:HG22	2:P:437:TYR:HB3	1.90	0.52
1:E:98:THR:O	1:E:102:GLY:CA	2.56	0.52
2:R:304:ASP:HB2	2:R:343:ILE:HB	1.92	0.52
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.92	0.52
2:M:497:ASN:HD22	2:M:497:ASN:C	2.14	0.52
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.24	0.51
1:A:176:GLU:HG3	1:A:180:LYS:C	2.30	0.51
1:F:188:ARG:HG3	1:F:188:ARG:NH1	2.25	0.51
2:N:390:LYS:HD2	6:N:743:HOH:O	2.10	0.51
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.45	0.51
1:E:62:LEU:HD13	1:E:101:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.74	0.51
1:C:163:GLN:HB2	6:C:819:HOH:O	2.10	0.51
1:B:6:PRO:HB2	2:N:503:GLN:NE2	2.26	0.51
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.93	0.51
1:D:51:LEU:HD11	1:D:126:ILE:HD12	1.91	0.51
1:D:1:PRO:HG2	2:R:488:MET:HE1	1.93	0.51
1:E:133:ARG:HG3	2:Q:326:THR:HG21	1.93	0.50
1:E:31:ARG:HB2	1:E:34:GLU:OE2	2.11	0.50
2:N:361:HIS:ND1	4:N:601:BME:H21	2.26	0.50
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.11	0.50
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.93	0.50
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.75	0.50
2:R:473:LYS:HD2	2:R:474:LEU:N	2.27	0.50
1:C:98:THR:O	1:C:102:GLY:HA2	2.12	0.50
1:E:165:GLN:NE2	1:E:165:GLN:N	2.21	0.50
1:F:176:GLU:HA	1:F:180:LYS:O	2.11	0.50
2:Q:399:MET:HA	2:Q:462:HIS:O	2.12	0.50
1:A:191:GLY:O	1:A:194:GLU:HB2	2.10	0.50
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.94	0.50
1:E:62:LEU:CD1	1:E:101:ALA:O	2.59	0.50
1:A:160:LEU:HD12	2:M:339:ILE:HG22	1.93	0.50
1:C:33:GLN:OE1	2:O:355:GLY:N	2.34	0.50
1:B:140:HIS:O	1:B:197:PHE:HA	2.12	0.50
1:B:28:ASN:HB3	1:B:29:PRO:HD2	1.93	0.50
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.26	0.50
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.47	0.50
2:O:497:ASN:HD22	2:O:499:GLU:H	1.58	0.50
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.94	0.50
1:F:19:ILE:O	2:R:426:VAL:HG21	2.12	0.50
2:R:383:ARG:HA	2:R:435:GLY:O	2.12	0.50
2:P:400:TRP:HA	2:P:425:GLY:O	2.11	0.49
1:A:33:GLN:HB3	1:A:85:LEU:CD1	2.42	0.49
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.32	0.49
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.94	0.49
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.47	0.49
1:D:177:VAL:HG12	1:D:178:ASP:OD2	2.11	0.49
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.94	0.49
2:R:432:ASP:OD1	2:R:434:ASP:N	2.45	0.49
2:R:385:VAL:O	2:R:526:VAL:HA	2.12	0.49
1:E:50:LEU:O	1:E:182:ALA:HA	2.13	0.49
1:A:54:GLN:HG2	1:A:102:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.12	0.49
2:M:376:GLU:O	2:M:442:ILE:HA	2.12	0.49
2:N:390:LYS:HD3	6:N:743:HOH:O	2.10	0.49
1:E:161:ILE:HD13	1:E:196:VAL:HG21	1.95	0.49
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.95	0.49
1:A:143:LEU:HD23	1:A:143:LEU:C	2.33	0.49
1:C:176:GLU:HA	1:C:180:LYS:O	2.13	0.49
1:D:165:GLN:H	1:D:165:GLN:HE21	1.59	0.49
1:E:84:ASN:HB3	1:E:87:ASN:ND2	2.27	0.49
1:F:48:HIS:C	1:F:180:LYS:HZ1	2.16	0.49
1:D:153:ALA:C	1:D:154:LYS:HE3	2.33	0.49
1:D:98:THR:O	1:D:102:GLY:HA2	2.12	0.49
2:P:313:ARG:O	2:P:318:LYS:HE3	2.12	0.48
1:D:114:VAL:HG23	1:D:122:MET:HE3	1.94	0.48
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.13	0.48
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.13	0.48
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.48	0.48
1:B:49:ILE:HD12	1:B:51:LEU:HD21	1.95	0.48
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.78	0.48
1:F:23:LEU:HB2	1:F:30:THR:HG22	1.96	0.48
2:M:400:TRP:HA	2:M:425:GLY:O	2.14	0.48
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.49	0.48
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.95	0.48
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.79	0.48
1:C:74:ASP:OD1	1:C:74:ASP:C	2.52	0.48
2:Q:404:ALA:HB2	2:Q:442:ILE:HD12	1.96	0.48
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.95	0.48
1:E:18:HIS:CE1	1:E:99:PHE:HE1	2.32	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.49	0.48
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.48	0.48
1:F:125:HIS:HA	1:F:143:LEU:O	2.14	0.48
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.49	0.48
1:C:24:GLU:O	1:C:27:GLY:N	2.43	0.48
1:E:114:VAL:HG23	1:E:122:MET:CE	2.44	0.48
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.82	0.48
2:Q:406:GLY:O	2:Q:447:TYR:HD1	1.97	0.48
1:F:49:ILE:N	1:F:180:LYS:HZ1	2.12	0.47
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.14	0.47
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.78	0.47
2:R:306:SER:OG	2:R:530:GLN:NE2	2.35	0.47
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.70	0.47
1:A:114:VAL:HG22	6:A:680:HOH:O	2.13	0.47
1:C:184:ARG:HG3	1:C:184:ARG:HH11	1.80	0.47
1:F:41:LYS:N	1:F:88:ALA:O	2.33	0.47
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.95	0.47
1:C:116:ASN:C	1:C:116:ASN:OD1	2.53	0.47
2:O:437:TYR:OH	2:O:523:PHE:HB3	2.15	0.47
1:B:69:GLU:OE2	1:B:94:ARG:HD3	2.15	0.47
1:C:114:VAL:HG23	1:C:122:MET:CE	2.44	0.47
1:E:177:VAL:O	1:E:180:LYS:HB3	2.14	0.47
1:E:176:GLU:HA	1:E:180:LYS:O	2.14	0.47
1:E:22:ALA:O	1:E:25:ALA:HB3	2.15	0.47
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.50	0.47
2:O:361:HIS:CD2	6:O:766:HOH:O	2.67	0.47
2:O:416:LEU:HD23	2:O:417:ALA:N	2.29	0.47
1:A:16:TYR:O	1:A:19:ILE:HG23	2.15	0.47
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.50	0.46
2:O:356:PHE:HD1	2:O:428:ARG:HD3	1.78	0.46
1:F:35:ILE:HD13	2:R:351:PHE:CE1	2.50	0.46
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.41	0.46
1:B:180:LYS:HD2	1:B:181:THR:N	2.30	0.46
1:F:190:GLN:NE2	2:R:331:SER:O	2.31	0.46
2:O:403:ASN:HB2	6:O:620:HOH:O	2.15	0.46
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	1.98	0.46
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.66	0.46
2:P:359:HIS:O	2:P:366:ASN:HB3	2.15	0.46
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.51	0.46
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.98	0.46
1:B:19:ILE:HD11	2:N:408:TYR:CD1	2.48	0.46
1:F:41:LYS:HE3	1:F:85:LEU:O	2.15	0.46
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.16	0.46
1:D:176:GLU:OE2	1:D:179:GLY:HA2	2.16	0.46
1:F:18:HIS:CE1	1:F:99:PHE:CE1	3.02	0.46
1:C:19:ILE:HG12	2:O:400:TRP:HB2	1.98	0.46
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.84	0.46
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.98	0.46
1:B:64:ARG:NE	1:B:100:ASP:O	2.45	0.46
1:F:64:ARG:HH11	1:F:64:ARG:HD2	1.26	0.45
2:M:416:LEU:HD23	2:M:416:LEU:C	2.36	0.45
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.98	0.45
1:A:50:LEU:O	1:A:182:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:HH11	1:B:64:ARG:HD2	1.33	0.45
1:D:19:ILE:CG2	2:P:410:HIS:HB2	2.47	0.45
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.75	0.45
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.51	0.45
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.97	0.45
2:N:414:ARG:HD2	2:N:414:ARG:HH11	1.49	0.45
2:Q:383:ARG:N	2:Q:524:ASP:OD1	2.46	0.45
2:R:392:VAL:HG12	2:R:395:THR:HB	1.99	0.45
1:C:58:GLY:HA3	1:C:190:GLN:OE1	2.15	0.45
1:F:37:ASN:HB2	1:F:106:LEU:HD12	1.97	0.45
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.98	0.45
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.51	0.45
1:C:3:GLU:HA	1:C:3:GLU:OE1	2.17	0.45
2:P:308:PHE:CE2	2:P:530:GLN:HB2	2.52	0.45
1:C:64:ARG:NE	1:C:100:ASP:O	2.38	0.45
1:C:131:PHE:O	1:C:132:ALA:CB	2.61	0.45
1:F:160:LEU:HA	1:F:160:LEU:HD23	1.77	0.45
1:D:176:GLU:HA	1:D:180:LYS:O	2.17	0.45
1:F:134:GLY:HA3	2:R:326:THR:HG22	1.99	0.45
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.16	0.45
2:N:364:LEU:HD12	2:N:373:PRO:HG2	1.99	0.45
2:O:390:LYS:CD	6:O:677:HOH:O	2.65	0.45
2:Q:392:VAL:HG12	2:Q:395:THR:HB	1.98	0.45
2:P:335:ALA:HB1	2:R:325:LYS:HG2	1.98	0.45
2:R:437:TYR:C	2:R:437:TYR:CD1	2.91	0.45
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.45
1:D:191:GLY:O	1:D:194:GLU:HB2	2.16	0.45
2:P:522:ARG:NH2	2:P:524:ASP:OD1	2.50	0.45
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.99	0.45
1:B:35:ILE:HG21	1:B:92:PHE:CE2	2.52	0.44
1:A:99:PHE:HE2	2:M:411:LYS:HD2	1.82	0.44
2:P:437:TYR:C	2:P:437:TYR:CD1	2.91	0.44
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.71	0.44
1:B:50:LEU:O	1:B:182:ALA:HA	2.17	0.44
1:E:52:LEU:O	1:E:184:ARG:HA	2.17	0.44
2:Q:383:ARG:HG3	2:Q:436:TYR:CE1	2.52	0.44
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.99	0.44
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.75	0.44
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.17	0.44
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.99	0.44
1:D:154:LYS:N	1:D:154:LYS:HE3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:LEU:HD11	1:E:106:LEU:HD11	1.97	0.44
2:P:376:GLU:OE1	6:P:677:HOH:O	2.20	0.44
1:C:98:THR:C	1:C:100:ASP:H	2.20	0.44
2:M:508:LEU:HD23	2:P:488:MET:CE	2.48	0.44
2:R:372:LEU:HA	2:R:372:LEU:HD12	1.69	0.44
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.28	0.44
1:B:176:GLU:HA	1:B:180:LYS:O	2.18	0.44
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.72	0.44
1:F:81:ASP:N	1:F:81:ASP:OD1	2.51	0.44
2:O:393:PRO:HG2	2:O:393:PRO:O	2.18	0.44
2:N:356:PHE:CE2	2:N:428:ARG:HD3	2.51	0.44
2:O:497:ASN:HD22	2:O:498:PRO:CD	2.31	0.44
1:F:188:ARG:CG	1:F:188:ARG:NH1	2.79	0.43
1:F:33:GLN:HG2	1:F:85:LEU:HD12	2.00	0.43
2:N:376:GLU:O	2:N:442:ILE:HA	2.18	0.43
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.31	0.43
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.66	0.43
1:E:51:LEU:HD11	1:E:126:ILE:HD12	1.99	0.43
1:A:78:GLU:CG	2:M:301:PRO:CG	2.95	0.43
2:M:341:GLN:HB3	2:M:346:THR:CG2	2.48	0.43
2:M:364:LEU:HB2	2:M:440:ARG:HD3	2.00	0.43
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.83	0.43
2:O:497:ASN:HD22	2:O:498:PRO:N	2.16	0.43
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.73	0.43
2:R:522:ARG:HE	2:R:524:ASP:CG	2.20	0.43
1:B:165:GLN:CA	1:B:165:GLN:HE21	2.30	0.43
1:C:28:ASN:HB3	6:C:807:HOH:O	2.18	0.43
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.84	0.43
1:E:174:ARG:HB2	1:E:183:TYR:CE1	2.53	0.43
2:N:513:ALA:O	2:N:515:PRO:HD3	2.18	0.43
2:O:381:ALA:O	2:O:522:ARG:HA	2.18	0.43
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.52	0.43
1:A:31:ARG:NH1	2:M:428:ARG:HG2	2.33	0.43
1:A:15:PRO:HB3	1:A:133:ARG:HD2	2.01	0.43
1:B:165:GLN:CD	1:B:165:GLN:H	2.05	0.43
1:E:143:LEU:HD23	1:E:143:LEU:C	2.39	0.43
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.48	0.43
1:E:100:ASP:OD1	1:E:100:ASP:N	2.52	0.43
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.84	0.43
2:R:505:ILE:O	2:R:507:LYS:HE3	2.19	0.43
1:E:131:PHE:O	1:E:132:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:495:ILE:HG21	2:N:500:ALA:HB3	2.01	0.43
2:O:414:ARG:HH11	2:O:414:ARG:HD2	1.63	0.43
2:O:497:ASN:HD22	2:O:498:PRO:HD2	1.84	0.43
2:P:495:ILE:HG21	2:P:500:ALA:HB3	2.01	0.43
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	2.00	0.43
2:P:335:ALA:HB2	2:R:328:ILE:HD12	1.99	0.43
1:A:33:GLN:HB3	1:A:85:LEU:HD12	2.00	0.43
1:C:98:THR:C	1:C:100:ASP:N	2.72	0.43
1:F:80:GLN:O	1:F:91:SER:HB2	2.19	0.43
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.39	0.43
1:F:92:PHE:CG	2:R:349:PRO:HG3	2.54	0.43
1:C:184:ARG:NH1	1:C:184:ARG:HG3	2.34	0.43
2:P:405:GLY:HA3	6:P:686:HOH:O	2.18	0.43
2:P:495:ILE:CG2	2:P:500:ALA:HB3	2.48	0.43
2:R:460:HIS:HA	2:R:478:LEU:O	2.18	0.43
1:E:50:LEU:HD12	1:E:51:LEU:N	2.33	0.43
1:E:58:GLY:CA	1:E:190:GLN:HB3	2.49	0.43
2:M:484:PRO:O	2:M:487:PRO:HD2	2.19	0.43
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.66	0.43
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.82	0.42
1:A:24:GLU:O	1:A:27:GLY:N	2.45	0.42
1:A:64:ARG:HD2	1:A:64:ARG:HH11	1.34	0.42
1:B:80:GLN:O	1:B:91:SER:HB2	2.19	0.42
1:C:140:HIS:O	1:C:197:PHE:HA	2.19	0.42
1:E:176:GLU:HG3	1:E:180:LYS:O	2.19	0.42
1:E:33:GLN:OE1	2:Q:355:GLY:N	2.45	0.42
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.49	0.42
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	2.01	0.42
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.53	0.42
2:R:324:TYR:OH	5:R:550:INO:O1	2.21	0.42
1:E:8:THR:HA	1:E:9:PRO:HD3	1.87	0.42
2:M:385:VAL:O	2:M:526:VAL:HA	2.19	0.42
2:N:488:MET:CE	1:C:1:PRO:HG2	2.49	0.42
2:Q:416:LEU:CD2	2:Q:416:LEU:C	2.87	0.42
1:F:20:GLY:HA2	2:R:426:VAL:HG13	2.01	0.42
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.01	0.42
1:C:41:LYS:O	1:C:44:ALA:N	2.47	0.42
1:C:70:VAL:HG21	1:C:106:LEU:HD21	2.02	0.42
1:F:116:ASN:C	1:F:116:ASN:OD1	2.58	0.42
1:F:35:ILE:CD1	2:R:351:PHE:CE1	3.02	0.42
2:M:437:TYR:CD1	2:M:437:TYR:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:407:ARG:HD3	2:P:417:ALA:O	2.20	0.42
1:A:44:ALA:O	1:A:48:HIS:NE2	2.40	0.42
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.35	0.42
2:O:406:GLY:O	2:O:447:TYR:CD1	2.69	0.42
2:P:399:MET:HA	2:P:462:HIS:O	2.20	0.42
2:Q:302:ALA:HB1	2:Q:347:THR:CG2	2.50	0.42
2:Q:407:ARG:NH1	2:Q:417:ALA:O	2.46	0.42
2:R:450:ARG:HH11	2:R:450:ARG:HD2	1.55	0.42
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.48	0.42
1:D:19:ILE:HD13	1:D:19:ILE:HG21	1.76	0.42
2:O:410:HIS:ND1	2:O:411:LYS:N	2.68	0.42
2:R:513:ALA:O	2:R:515:PRO:HD3	2.20	0.42
1:C:161:ILE:CD1	1:C:196:VAL:HG11	2.50	0.42
1:F:19:ILE:O	2:R:426:VAL:CG2	2.68	0.42
1:A:165:GLN:H	1:A:165:GLN:NE2	2.18	0.42
1:A:110:LYS:HE2	1:A:148:GLU:OE2	2.20	0.41
1:C:164:PRO:HA	1:C:167:ARG:HD2	2.02	0.41
1:D:39:LEU:HD11	1:D:93:GLY:HA3	2.01	0.41
1:F:48:HIS:N	1:F:48:HIS:CD2	2.88	0.41
2:O:415:TYR:CE1	2:O:416:LEU:HD22	2.54	0.41
1:B:143:LEU:HD23	1:B:143:LEU:C	2.40	0.41
1:C:70:VAL:HG11	1:C:106:LEU:CD2	2.50	0.41
1:D:165:GLN:H	1:D:165:GLN:CD	2.23	0.41
1:E:116:ASN:OD1	1:E:116:ASN:C	2.59	0.41
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.86	0.41
2:O:519:LEU:HD23	2:O:519:LEU:HA	1.88	0.41
2:P:313:ARG:O	2:P:318:LYS:CE	2.68	0.41
1:D:25:ALA:O	2:P:411:LYS:NZ	2.34	0.41
1:F:74:ASP:HB3	1:F:89:PHE:CD2	2.55	0.41
2:O:478:LEU:C	2:O:478:LEU:HD23	2.40	0.41
2:R:443:LYS:HE2	2:R:480:PHE:CG	2.56	0.41
1:D:39:LEU:O	1:D:89:PHE:HA	2.21	0.41
2:N:495:ILE:CG2	2:N:500:ALA:HB3	2.49	0.41
1:E:92:PHE:CG	2:Q:349:PRO:HG3	2.55	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.87	0.41
1:A:114:VAL:HG23	1:A:122:MET:CE	2.51	0.41
1:D:19:ILE:HD11	2:P:408:TYR:CD2	2.43	0.41
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.50	0.41
1:F:120:VAL:HA	1:F:121:PRO:HD3	1.82	0.41
2:M:376:GLU:HG2	2:P:446:PRO:HD2	2.01	0.41
2:N:333:ARG:HH11	2:N:333:ARG:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:536:GLU:HB2	6:N:799:HOH:O	2.21	0.41
1:E:190:GLN:NE2	2:Q:331:SER:O	2.35	0.41
1:C:19:ILE:HG13	2:O:426:VAL:HG22	2.03	0.41
1:F:115:ASN:HA	1:F:121:PRO:HA	2.02	0.41
2:N:497:ASN:HA	2:N:498:PRO:HD3	1.87	0.41
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.78	0.41
1:C:176:GLU:HG3	1:C:180:LYS:C	2.41	0.41
1:E:58:GLY:HA2	1:E:190:GLN:HB3	2.03	0.41
2:M:359:HIS:O	2:M:366:ASN:HB3	2.20	0.41
1:B:35:ILE:HD13	2:N:351:PHE:CE1	2.55	0.41
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.77	0.41
2:N:522:ARG:NH1	6:N:767:HOH:O	2.21	0.41
2:M:310:ILE:CD1	2:O:453:PRO:HB2	2.45	0.41
1:A:198:PHE:HA	2:M:337:VAL:O	2.20	0.41
2:M:406:GLY:O	2:M:447:TYR:HD1	2.03	0.41
2:P:420:ASP:HA	2:P:421:PRO:HD2	1.94	0.41
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.72	0.41
2:Q:331:SER:HA	2:Q:332:PRO:HD3	1.82	0.41
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.56	0.41
1:E:188:ARG:CG	1:E:188:ARG:HH11	2.33	0.41
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.03	0.41
2:M:310:ILE:HD12	2:O:453:PRO:CB	2.47	0.41
2:N:420:ASP:HA	2:N:421:PRO:HD2	1.88	0.41
2:R:305:ASN:N	6:R:879:HOH:O	2.35	0.41
1:B:74:ASP:HB2	6:B:690:HOH:O	2.21	0.41
1:F:53:GLY:HA3	1:F:185:PHE:O	2.20	0.41
1:F:24:GLU:O	1:F:27:GLY:N	2.52	0.41
2:N:364:LEU:HD12	2:N:364:LEU:HA	1.88	0.41
2:R:312:ASP:C	2:R:312:ASP:OD1	2.60	0.41
1:B:70:VAL:HG21	1:B:106:LEU:HD21	2.04	0.40
1:C:39:LEU:O	1:C:89:PHE:HA	2.21	0.40
1:D:52:LEU:CD2	1:D:184:ARG:NH1	2.84	0.40
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.36	0.40
2:O:362:ASP:OD1	2:O:440:ARG:HD3	2.22	0.40
2:R:444:PRO:O	2:R:459:ALA:HB1	2.21	0.40
1:C:100:ASP:HB2	1:C:101:ALA:H	1.67	0.40
1:F:110:LYS:HE2	1:F:148:GLU:OE2	2.21	0.40
1:B:176:GLU:HG2	1:B:179:GLY:C	2.42	0.40
1:D:51:LEU:CD1	1:D:126:ILE:HD12	2.50	0.40
1:E:39:LEU:HD11	1:E:93:GLY:HA3	2.02	0.40
2:O:392:VAL:HG12	2:O:395:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.36	0.40
1:B:39:LEU:HD11	1:B:93:GLY:HA3	2.04	0.40
1:E:38:ARG:HH11	1:E:38:ARG:HD2	1.68	0.40
2:Q:488:MET:CE	1:F:1:PRO:HG2	2.51	0.40
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.72	0.40
2:O:331:SER:HA	2:O:332:PRO:HD3	1.94	0.40
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.21	0.40
2:Q:438:SER:O	4:Q:601:BME:H21	2.21	0.40
1:A:64:ARG:NE	1:A:100:ASP:O	2.50	0.40
2:O:473:LYS:HD3	6:O:783: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%)	188 (95%)	10 (5%)	0	100	100
1	B	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	C	198/200 (99%)	189 (96%)	8 (4%)	1 (0%)	29	22
1	D	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	29	22
2	M	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	N	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	224 (98%)	5 (2%)	0	100	100
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2562/2628 (98%)	2455 (96%)	105 (4%)	2 (0%)	51	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	ALA
1	F	74	ASP

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%)	153 (94%)	9 (6%)	21	16
1	B	162/163 (99%)	154 (95%)	8 (5%)	25	20
1	C	162/163 (99%)	155 (96%)	7 (4%)	29	25
1	D	162/163 (99%)	154 (95%)	8 (5%)	25	20
1	E	162/163 (99%)	153 (94%)	9 (6%)	21	16
1	F	162/163 (99%)	155 (96%)	7 (4%)	29	25
2	M	196/202 (97%)	183 (93%)	13 (7%)	16	11
2	N	196/202 (97%)	189 (96%)	7 (4%)	35	32
2	O	196/202 (97%)	184 (94%)	12 (6%)	18	13
2	P	196/202 (97%)	184 (94%)	12 (6%)	18	13
2	Q	196/202 (97%)	186 (95%)	10 (5%)	24	19
2	R	196/202 (97%)	185 (94%)	11 (6%)	21	16
All	All	2148/2190 (98%)	2035 (95%)	113 (5%)	22	18

All (113) 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	38	ARG
1	A	42	PRO
1	A	52	LEU
1	A	91	SER
1	A	100	ASP
1	A	165	GLN
1	A	188	ARG
2	M	301	PRO
2	M	326	THR
2	M	372	LEU
2	M	395	THR
2	M	411	LYS
2	M	416	LEU
2	M	428	ARG
2	M	434	ASP
2	M	488	MET
2	M	497	ASN
2	M	507	LYS
2	M	512	ASN
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	42	PRO
1	B	52	LEU
1	B	64	ARG
1	B	100	ASP
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	416	LEU
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	100	ASP
1	C	154	LYS
1	C	165	GLN

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Mol	Chain	Res	Type
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	428	ARG
2	O	433	SER
2	O	434	ASP
2	O	478	LEU
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	100	ASP
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	411	LYS
2	P	416	LEU
2	P	428	ARG
2	P	434	ASP
2	P	442	ILE
2	P	478	LEU
2	P	497	ASN
2	P	503	GLN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU
1	E	100	ASP
1	E	165	GLN
1	E	178	ASP
1	E	180	LYS
1	E	181	THR
2	Q	364	LEU

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Mol	Chain	Res	Type
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	438	SER
2	Q	478	LEU
2	Q	497	ASN
2	Q	507	LYS
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	100	ASP
1	F	165	GLN
1	F	176	GLU
1	F	181	THR
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP
2	R	438	SER
2	R	473	LYS
2	R	478	LEU
2	R	497	ASN
2	R	507	LYS
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN

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Mol	Chain	Res	Type
2	N	534	HIS
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
1	D	18	HIS
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	18	HIS
1	E	165	GLN
2	Q	361	HIS
2	Q	497	ASN
2	Q	503	GLN
1	F	165	GLN
2	R	361	HIS
2	R	497	ASN
2	R	503	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
5	INO	Q	550	3	6,11,11	3.07	3 (50%)	7,15,15	1.11	0
5	INO	R	550	3	6,11,11	2.89	2 (33%)	7,15,15	0.69	0
5	INO	P	550	3	6,11,11	3.46	2 (33%)	7,15,15	0.91	0
4	BME	O	601	2	3,3,3	0.54	0	1,2,2	1.04	0
4	BME	N	601	2	3,3,3	0.62	0	1,2,2	1.54	0
5	INO	M	550	3	6,11,11	3.43	2 (33%)	7,15,15	0.72	0
5	INO	N	550	3	6,11,11	3.10	2 (33%)	7,15,15	0.83	0
5	INO	O	550	3	6,11,11	3.23	3 (50%)	7,15,15	1.03	0
4	BME	Q	601	2	3,3,3	1.00	0	1,2,2	1.46	0
4	BME	P	601	2	3,3,3	0.76	0	1,2,2	2.26	1 (100%)
4	BME	R	601	2	3,3,3	0.39	0	1,2,2	0.97	0
4	BME	M	601	2	3,3,3	0.70	0	1,2,2	1.43	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
5	INO	Q	550	3	-	0/0/4/4	0/1/1/1
5	INO	R	550	3	-	0/0/4/4	0/1/1/1
5	INO	P	550	3	-	0/0/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	-
4	BME	N	601	2	-	1/1/1/1	-
5	INO	M	550	3	-	0/0/4/4	0/1/1/1
5	INO	N	550	3	-	0/0/4/4	0/1/1/1
5	INO	O	550	3	-	0/0/4/4	0/1/1/1
4	BME	Q	601	2	-	1/1/1/1	-
4	BME	P	601	2	-	0/1/1/1	-
4	BME	R	601	2	-	1/1/1/1	-
4	BME	M	601	2	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	INO	C4-C7	7.75	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550	INO	C4-C7	7.55	1.54	1.47
5	O	550	INO	C4-C7	7.14	1.54	1.47
5	N	550	INO	C4-C7	6.76	1.54	1.47
5	Q	550	INO	C4-C7	6.59	1.53	1.47
5	R	550	INO	C4-C7	5.86	1.53	1.47
5	R	550	INO	O3-C2	-3.18	1.23	1.32
5	N	550	INO	O3-C2	-3.00	1.23	1.32
5	M	550	INO	O3-C2	-2.95	1.24	1.32
5	P	550	INO	O3-C2	-2.84	1.24	1.32
5	Q	550	INO	C3-C4	2.46	1.44	1.39
5	O	550	INO	O3-C2	-2.33	1.25	1.32
5	Q	550	INO	O3-C2	-2.28	1.25	1.32
5	O	550	INO	C3-C4	2.13	1.43	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	601	BME	O1-C1-C2	-2.26	101.92	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	601	BME	O1-C1-C2-S2
4	Q	601	BME	O1-C1-C2-S2
4	R	601	BME	O1-C1-C2-S2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	550	INO	1	0
4	N	601	BME	1	0
4	Q	601	BME	1	0

5.7 Other polymers [i](#)

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.