



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 AM UTC

PDB ID : 3PCD / pdb_00003pcd
Title : PROTOCATECHUATE 3,4-DIOXYGENASE Y447H MUTANT
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-11-24
Resolution : 2.10 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

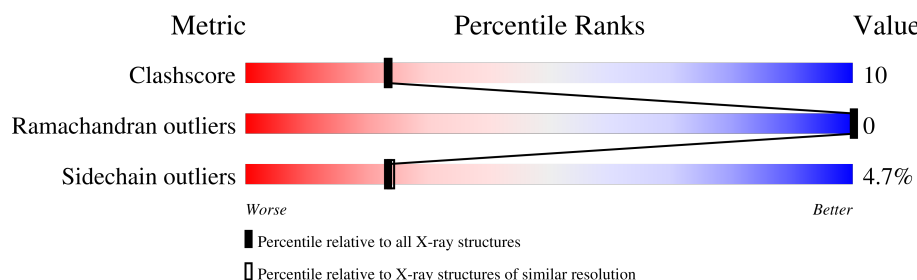
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	76% 20% . .
1	B	200	79% 16% . .
1	C	200	70% 26% .
1	D	200	75% 20% .
1	E	200	68% 26% 6%
1	F	200	66% 22% 10%
2	M	238	70% 21% 7% .
2	N	238	78% 18% . .

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Mol	Chain	Length	Quality of chain
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CO3	Q	550	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21930 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
			1838	1168	336	327	7			
2	N	233	Total	C	N	O	S	0	0	0
			1838	1168	336	327	7			
2	O	233	Total	C	N	O	S	0	0	0
			1838	1168	336	327	7			
2	P	233	Total	C	N	O	S	0	0	0
			1838	1168	336	327	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1838	1168	336	327	7			
2	R	233	Total	C	N	O	S	0	0	0
			1838	1168	336	327	7			

There are 6 discrepancies between the modelled and reference sequences:

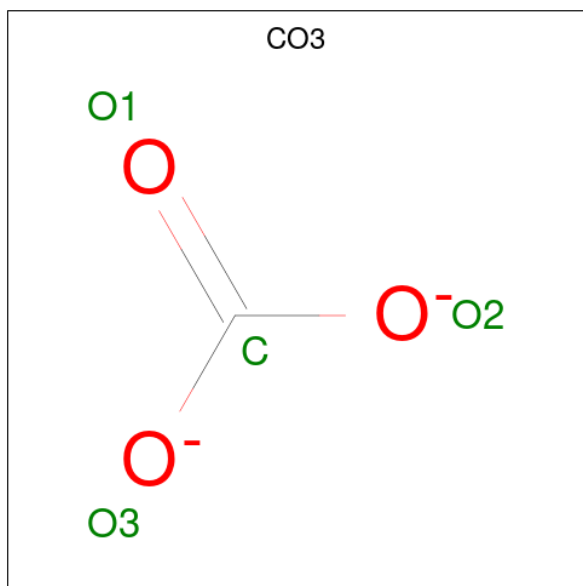
Chain	Residue	Modelled	Actual	Comment	Reference
M	447	HIS	TYR	engineered mutation	UNP P00437

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Chain	Residue	Modelled	Actual	Comment	Reference
N	447	HIS	TYR	engineered mutation	UNP P00437
O	447	HIS	TYR	engineered mutation	UNP P00437
P	447	HIS	TYR	engineered mutation	UNP P00437
Q	447	HIS	TYR	engineered mutation	UNP P00437
R	447	HIS	TYR	engineered mutation	UNP P00437

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

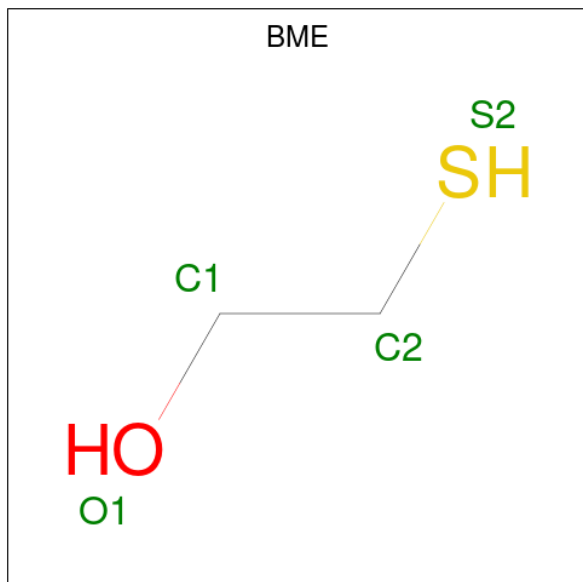


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			4	1	3		
3	N	1	Total	C	O	0	0
			4	1	3		
3	O	1	Total	C	O	0	0
			4	1	3		
3	P	1	Total	C	O	0	0
			4	1	3		
3	Q	1	Total	C	O	0	0
			4	1	3		
3	R	1	Total	C	O	0	0
			4	1	3		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 5 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 6 is water.

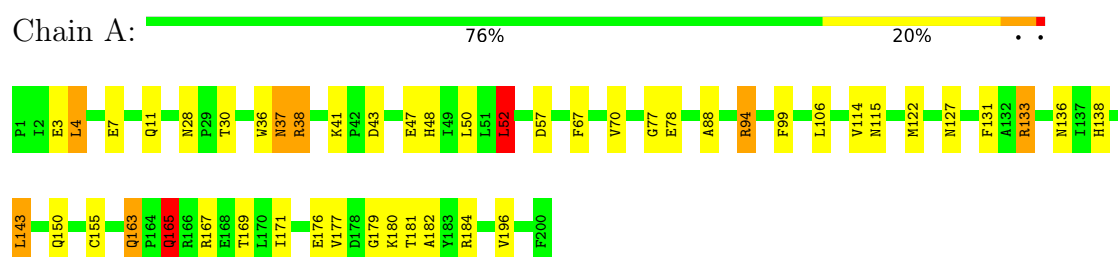
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total 73	O 73	0	0
6	M	161	Total 161	O 161	0	0
6	B	79	Total 79	O 79	0	0
6	N	163	Total 163	O 163	0	0
6	C	78	Total 78	O 78	0	0
6	O	156	Total 156	O 156	0	0
6	D	81	Total 81	O 81	0	0
6	P	151	Total 151	O 151	0	0
6	E	82	Total 82	O 82	0	0
6	Q	159	Total 159	O 159	0	0
6	F	80	Total 80	O 80	0	0
6	R	159	Total 159	O 159	0	0

3 Residue-property plots [i](#)

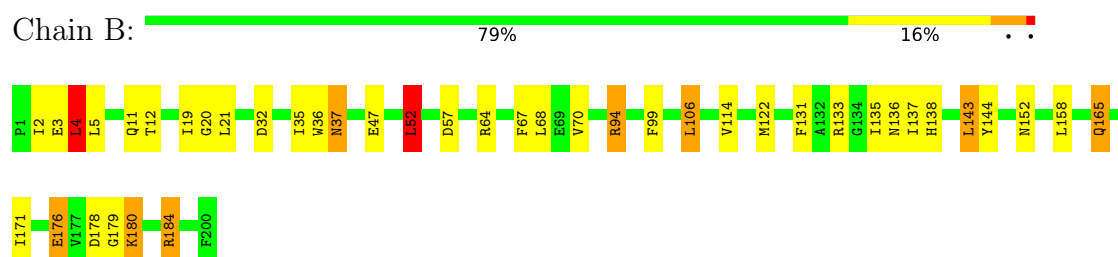
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

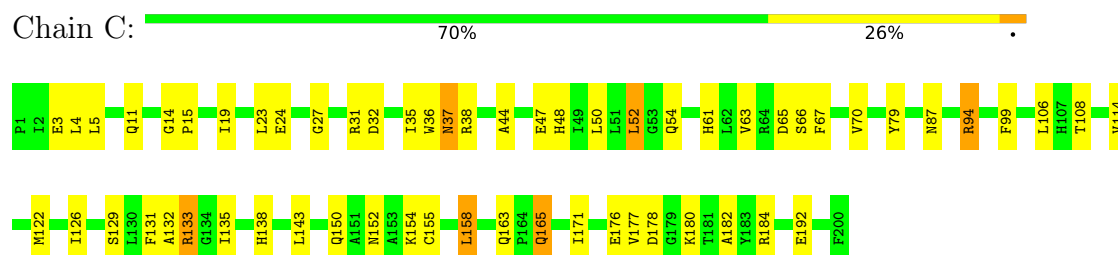
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



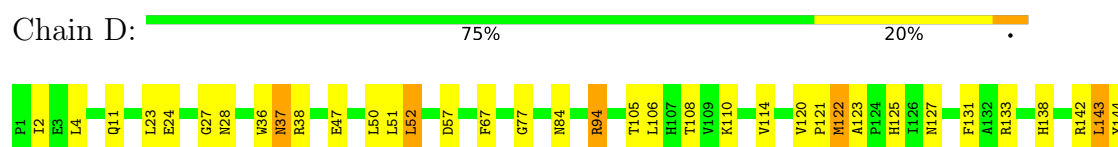
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

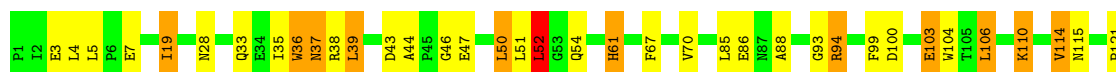




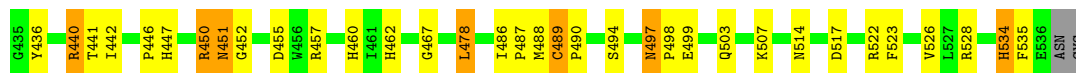
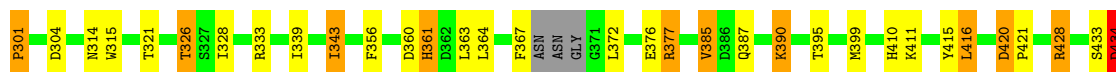
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



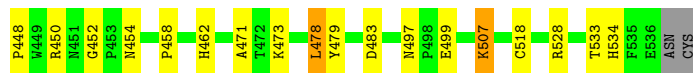
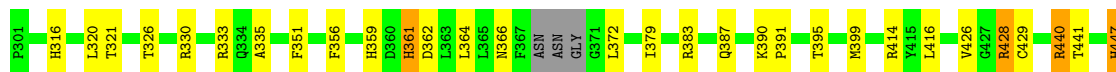
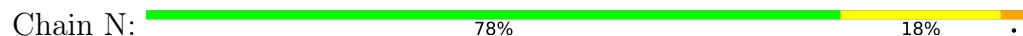
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



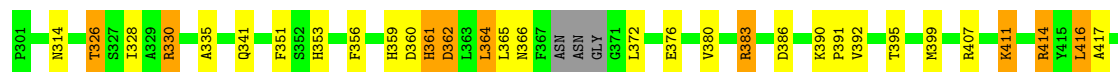
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 70% 21% 6% ..



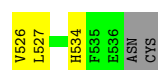
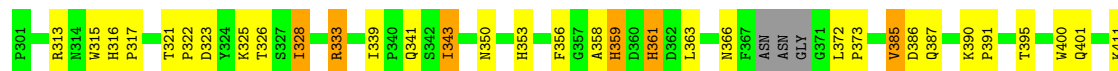
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 68% 25% ..



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 68% 24% 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	197.40Å 127.20Å 134.60Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.0 (6.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21930	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: CO3, BME, FE

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	1.34	2/1611 (0.1%)	1.86	31/2195 (1.4%)
1	B	1.34	6/1611 (0.4%)	1.90	24/2195 (1.1%)
1	C	1.35	5/1611 (0.3%)	1.77	25/2195 (1.1%)
1	D	1.35	6/1611 (0.4%)	1.93	24/2195 (1.1%)
1	E	1.33	5/1611 (0.3%)	1.80	26/2195 (1.2%)
1	F	1.34	1/1611 (0.1%)	1.85	35/2195 (1.6%)
2	M	1.46	7/1893 (0.4%)	1.85	37/2577 (1.4%)
2	N	1.40	5/1893 (0.3%)	1.79	26/2577 (1.0%)
2	O	1.44	7/1893 (0.4%)	1.87	31/2577 (1.2%)
2	P	1.48	6/1893 (0.3%)	1.84	36/2577 (1.4%)
2	Q	1.50	9/1893 (0.5%)	1.87	39/2577 (1.5%)
2	R	1.47	7/1893 (0.4%)	1.87	42/2577 (1.6%)
All	All	1.41	66/21024 (0.3%)	1.85	376/28632 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	P	0	1
All	All	0	2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	ARG	CD-NE	-8.38	1.34	1.46
1	A	94	ARG	CD-NE	-8.29	1.34	1.46
2	R	321	THR	N-CA	8.25	1.55	1.46
2	R	452	GLY	N-CA	8.19	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	451	ASN	CA-C	8.01	1.56	1.52
2	P	451	ASN	CA-C	7.96	1.56	1.52
2	N	441	THR	CA-CB	7.50	1.63	1.53
2	Q	440	ARG	CD-NE	-7.43	1.35	1.46
2	P	428	ARG	CD-NE	-7.37	1.35	1.46
2	M	321	THR	N-CA	7.18	1.55	1.46
2	N	440	ARG	CD-NE	-7.03	1.36	1.46
2	Q	428	ARG	CD-NE	-6.98	1.36	1.46
2	M	451	ASN	CA-C	6.89	1.55	1.52
1	D	133	ARG	CD-NE	-6.84	1.36	1.46
2	O	477	GLN	C-O	6.60	1.31	1.23
2	N	428	ARG	CD-NE	-6.54	1.37	1.46
1	D	108	THR	CA-CB	6.42	1.63	1.54
2	Q	441	THR	CA-CB	6.36	1.62	1.54
1	B	94	ARG	CD-NE	-6.29	1.37	1.46
2	M	452	GLY	N-CA	6.14	1.53	1.44
2	O	339	ILE	CA-CB	6.09	1.62	1.54
2	R	428	ARG	CD-NE	-6.08	1.37	1.46
2	R	401	GLN	C-O	6.08	1.30	1.23
1	E	94	ARG	CD-NE	-6.03	1.37	1.46
2	M	440	ARG	CD-NE	-6.03	1.37	1.46
2	O	440	ARG	CD-NE	-6.01	1.37	1.46
2	N	429	CYS	N-CA	6.00	1.53	1.46
1	C	14	GLY	N-CA	5.98	1.52	1.44
2	M	523	PHE	N-CA	5.94	1.53	1.46
2	O	506	ALA	N-CA	5.79	1.53	1.46
1	B	137	ILE	CB-CG1	5.76	1.65	1.53
2	P	362	ASP	N-CA	5.67	1.53	1.46
1	B	133	ARG	NE-CZ	-5.65	1.26	1.33
1	C	129	SER	C-N	-5.64	1.25	1.33
2	N	321	THR	N-CA	5.57	1.52	1.46
2	O	310	ILE	CA-CB	5.56	1.59	1.54
2	Q	495	ILE	CA-CB	5.54	1.60	1.54
1	D	2	ILE	CA-CB	5.53	1.61	1.54
1	E	5	LEU	CA-C	5.46	1.59	1.53
2	R	385	VAL	N-CA	5.40	1.52	1.46
2	R	440	ARG	CD-NE	-5.40	1.38	1.46
1	F	36	TRP	CA-C	-5.37	1.48	1.53
2	M	441	THR	CA-CB	5.32	1.60	1.53
1	B	2	ILE	CA-CB	5.31	1.60	1.54
2	Q	458	PRO	C-O	5.31	1.30	1.23
1	C	108	THR	CA-CB	5.30	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	445	GLY	N-CA	5.28	1.51	1.44
1	B	11	GLN	C-O	5.28	1.30	1.23
2	M	452	GLY	CA-C	5.27	1.59	1.51
1	A	196	VAL	CA-C	5.22	1.58	1.52
2	Q	452	GLY	N-CA	5.21	1.51	1.44
1	D	123	ALA	N-CA	5.21	1.53	1.45
1	B	133	ARG	CD-NE	-5.21	1.39	1.46
1	E	123	ALA	N-CA	5.19	1.52	1.45
2	O	451	ASN	N-CA	5.18	1.52	1.46
2	Q	527	LEU	N-CA	5.16	1.51	1.45
2	P	440	ARG	CA-C	5.15	1.58	1.52
2	R	430	LEU	N-CA	5.12	1.52	1.46
1	C	94	ARG	CD-NE	-5.11	1.39	1.46
1	C	11	GLN	CA-C	5.11	1.58	1.52
2	Q	336	LEU	N-CA	5.10	1.52	1.46
1	E	108	THR	CA-CB	5.09	1.61	1.54
1	D	125	HIS	CE1-NE2	5.04	1.37	1.32
2	P	330	ARG	CD-NE	-5.02	1.39	1.46
2	P	506	ALA	C-O	5.01	1.30	1.23
1	E	90	ASN	CA-C	5.01	1.58	1.52

All (376) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ARG	CD-NE-CZ	29.95	166.32	124.40
1	B	133	ARG	CD-NE-CZ	29.40	165.56	124.40
1	A	94	ARG	CD-NE-CZ	16.44	147.42	124.40
2	P	440	ARG	NE-CZ-NH2	-16.38	104.46	119.20
1	C	133	ARG	CD-NE-CZ	14.60	144.83	124.40
1	E	133	ARG	CD-NE-CZ	13.80	143.72	124.40
1	A	133	ARG	CD-NE-CZ	12.84	142.38	124.40
2	O	353	HIS	CA-CB-CG	-12.77	101.03	113.80
1	D	94	ARG	CD-NE-CZ	12.55	141.97	124.40
1	D	47	GLU	CA-CB-CG	11.90	137.90	114.10
2	N	440	ARG	NE-CZ-NH2	-11.51	108.84	119.20
2	N	452	GLY	N-CA-C	-11.08	98.83	112.23
2	P	428	ARG	CG-CD-NE	10.78	135.72	112.00
2	R	428	ARG	CD-NE-CZ	10.75	139.46	124.40
2	M	452	GLY	N-CA-C	-10.60	99.41	112.23
2	O	452	GLY	N-CA-C	-10.42	99.63	112.23
1	A	115	ASN	CA-CB-CG	10.29	122.89	112.60
2	R	440	ARG	NE-CZ-NH2	-10.11	110.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	440	ARG	NE-CZ-NH2	-10.10	110.11	119.20
1	B	176	GLU	CB-CG-CD	10.09	129.75	112.60
1	D	94	ARG	CG-CD-NE	10.06	134.14	112.00
2	P	353	HIS	CA-CB-CG	-9.99	103.81	113.80
2	Q	428	ARG	CD-NE-CZ	9.96	138.34	124.40
2	R	361	HIS	CA-CB-CG	-9.93	103.87	113.80
2	P	440	ARG	NE-CZ-NH1	9.90	131.40	121.50
1	A	136	ASN	OD1-CG-ND2	9.87	132.47	122.60
2	R	387	GLN	OE1-CD-NE2	9.86	132.46	122.60
1	F	177	VAL	CB-CA-C	9.84	122.44	110.73
1	C	94	ARG	NE-CZ-NH2	-9.71	110.46	119.20
2	R	452	GLY	N-CA-C	-9.56	100.66	112.23
1	F	47	GLU	CA-CB-CG	9.53	133.16	114.10
1	D	94	ARG	NE-CZ-NH2	-9.48	110.67	119.20
2	Q	452	GLY	N-CA-C	-9.29	100.98	112.23
2	O	434	ASP	CA-CB-CG	-9.16	103.44	112.60
2	Q	451	ASN	O-C-N	9.16	127.61	120.83
1	C	47	GLU	CA-CB-CG	9.08	132.26	114.10
2	M	450	ARG	CD-NE-CZ	9.05	137.07	124.40
2	P	452	GLY	N-CA-C	-9.01	101.02	112.10
2	P	428	ARG	CD-NE-CZ	8.95	136.93	124.40
2	P	451	ASN	O-C-N	8.94	127.44	120.83
2	Q	457	ARG	NE-CZ-NH1	8.91	130.41	121.50
1	B	184	ARG	NE-CZ-NH2	-8.90	111.19	119.20
2	M	489	CYS	O-C-N	8.70	128.71	121.31
1	A	94	ARG	CG-CD-NE	8.64	131.02	112.00
2	N	428	ARG	CG-CD-NE	8.62	130.96	112.00
2	O	447	HIS	O-C-N	8.55	130.78	122.06
2	M	434	ASP	CA-CB-CG	-8.42	104.18	112.60
1	C	94	ARG	CD-NE-CZ	8.26	135.96	124.40
1	F	43	ASP	CA-CB-CG	-8.25	104.35	112.60
1	D	37	ASN	N-CA-C	8.16	122.86	113.15
1	A	94	ARG	CB-CG-CD	8.08	129.89	111.30
2	R	450	ARG	CD-NE-CZ	-8.08	113.09	124.40
1	C	94	ARG	NE-CZ-NH1	8.06	129.56	121.50
2	M	528	ARG	CA-C-N	8.05	127.65	119.92
2	M	528	ARG	C-N-CA	8.05	127.65	119.92
2	Q	325	LYS	N-CA-C	7.93	120.93	111.33
1	B	47	GLU	CA-CB-CG	7.92	129.94	114.10
2	O	361	HIS	CA-CB-CG	-7.83	105.97	113.80
2	N	387	GLN	OE1-CD-NE2	7.75	130.35	122.60
2	Q	311	ARG	CD-NE-CZ	7.72	135.21	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	ASN	CA-CB-CG	-7.71	104.89	112.60
1	B	137	ILE	CB-CA-C	7.70	121.56	110.33
1	D	94	ARG	CB-CG-CD	7.62	128.83	111.30
1	B	37	ASN	N-CA-C	7.57	121.41	112.93
1	F	163	GLN	CA-C-O	7.56	124.91	119.32
1	E	37	ASN	N-CA-C	7.54	122.08	113.02
2	Q	361	HIS	CA-CB-CG	-7.53	106.27	113.80
1	B	94	ARG	CG-CD-NE	7.44	128.37	112.00
1	B	99	PHE	N-CA-C	-7.43	103.12	111.07
1	C	133	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	F	28	ASN	O-C-N	7.41	127.64	121.35
1	B	178	ASP	CB-CA-C	7.37	122.36	111.89
2	Q	434	ASP	CA-CB-CG	-7.35	105.25	112.60
2	M	428	ARG	CD-NE-CZ	7.34	134.68	124.40
2	Q	440	ARG	NE-CZ-NH2	-7.31	112.62	119.20
2	R	440	ARG	NH1-CZ-NH2	7.29	128.77	119.30
1	E	94	ARG	CG-CD-NE	7.26	127.97	112.00
2	O	440	ARG	NE-CZ-NH2	-7.26	112.67	119.20
2	M	361	HIS	CA-CB-CG	-7.20	106.60	113.80
1	E	163	GLN	CA-C-O	7.19	124.64	119.32
2	Q	454	ASN	CA-CB-CG	7.19	119.79	112.60
1	B	94	ARG	NE-CZ-NH1	7.18	128.68	121.50
2	O	454	ASN	CA-CB-CG	7.12	119.72	112.60
1	F	7	GLU	CB-CG-CD	7.06	124.61	112.60
2	P	386	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	99	PHE	N-CA-C	-7.05	103.60	111.71
2	M	411	LYS	CB-CA-C	-7.04	99.05	110.74
2	N	447	HIS	CA-CB-CG	-7.04	106.76	113.80
1	A	7	GLU	CB-CG-CD	7.03	124.54	112.60
1	F	166	ARG	NE-CZ-NH2	-7.01	112.89	119.20
2	N	507	LYS	CA-CB-CG	6.97	128.05	114.10
1	D	28	ASN	O-C-N	6.97	127.28	121.35
2	R	350	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	E	64	ARG	CD-NE-CZ	-6.95	114.67	124.40
1	E	5	LEU	O-C-N	6.94	129.16	121.53
1	D	158	LEU	CB-CA-C	6.91	122.27	110.79
2	R	428	ARG	CB-CG-CD	6.87	127.09	111.30
2	R	353	HIS	CA-CB-CG	-6.86	106.94	113.80
1	D	127	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	C	94	ARG	CB-CG-CD	6.82	126.98	111.30
1	E	165	GLN	CB-CG-CD	6.81	124.18	112.60
2	R	473	LYS	CA-CB-CG	6.79	127.69	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	454	ASN	CA-CB-CG	6.76	119.36	112.60
2	P	361	HIS	CA-CB-CG	-6.73	107.07	113.80
1	D	177	VAL	CB-CA-C	6.71	118.71	110.73
1	A	171	ILE	N-CA-C	6.70	117.49	107.51
1	A	127	ASN	CA-CB-CG	-6.68	105.92	112.60
2	Q	442	ILE	CA-CB-CG2	6.67	121.84	110.50
1	E	5	LEU	N-CA-C	-6.67	100.88	110.08
1	E	28	ASN	O-C-N	6.65	127.00	121.35
1	D	11	GLN	O-C-N	6.64	130.81	123.25
2	P	428	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	F	86	GLU	CB-CG-CD	6.60	123.82	112.60
1	B	94	ARG	CB-CG-CD	6.59	126.46	111.30
2	R	434	ASP	CA-CB-CG	-6.57	106.03	112.60
2	M	457	ARG	CD-NE-CZ	6.56	133.59	124.40
2	P	458	PRO	CB-CA-C	-6.55	102.36	110.95
2	P	484	PRO	CB-CA-C	6.55	121.15	111.85
1	B	47	GLU	CB-CA-C	-6.55	100.71	110.67
1	D	38	ARG	CD-NE-CZ	6.55	133.56	124.40
2	R	428	ARG	CG-CD-NE	6.50	126.31	112.00
2	Q	522	ARG	NE-CZ-NH1	-6.48	115.02	121.50
1	A	165	GLN	CB-CG-CD	6.48	123.61	112.60
1	F	171	ILE	N-CA-C	6.45	118.09	108.23
1	C	37	ASN	N-CA-C	6.43	120.73	113.02
1	B	152	ASN	CA-CB-CG	6.42	119.03	112.60
1	E	94	ARG	CB-CG-CD	6.41	126.04	111.30
2	O	387	GLN	OE1-CD-NE2	6.38	128.98	122.60
2	R	451	ASN	OD1-CG-ND2	6.37	128.97	122.60
2	R	328	ILE	N-CA-C	6.34	116.51	110.42
1	C	99	PHE	N-CA-C	-6.34	104.37	111.28
2	O	350	ASN	OD1-CG-ND2	-6.33	116.27	122.60
2	N	428	ARG	CB-CG-CD	6.33	125.86	111.30
2	N	428	ARG	NE-CZ-NH1	6.32	127.82	121.50
1	C	87	ASN	CA-CB-CG	6.32	118.92	112.60
2	M	367	PHE	CA-C-O	-6.31	110.07	120.80
2	R	411	LYS	CB-CA-C	-6.30	100.28	110.74
2	R	525	ILE	O-C-N	6.29	129.83	123.10
1	F	140	HIS	CB-CA-C	-6.28	99.39	109.75
2	Q	440	ARG	CD-NE-CZ	6.27	133.18	124.40
2	Q	457	ARG	NE-CZ-NH2	-6.27	113.56	119.20
2	Q	428	ARG	NE-CZ-NH2	-6.25	113.58	119.20
2	Q	411	LYS	CB-CA-C	-6.25	100.47	110.84
2	M	451	ASN	O-C-N	6.21	125.42	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	467	GLY	O-C-N	6.20	127.97	121.77
2	Q	481	GLU	CB-CG-CD	6.19	123.12	112.60
1	D	94	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	D	185	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	150	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	A	57	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	64	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	F	94	ARG	NE-CZ-NH2	-6.13	113.69	119.20
1	F	185	PHE	CA-CB-CG	6.12	119.92	113.80
2	M	420	ASP	CB-CA-C	6.10	116.21	110.17
1	F	3	GLU	O-C-N	6.09	130.44	123.31
1	F	5	LEU	N-CA-C	-6.09	102.10	109.83
2	Q	512	ASN	CA-CB-CG	-6.09	106.51	112.60
2	M	314	ASN	N-CA-C	-6.08	106.02	113.50
1	C	11	GLN	N-CA-CB	6.06	122.23	111.69
2	O	497	ASN	CB-CA-C	6.05	118.09	109.38
2	R	412	ASN	CA-CB-CG	6.04	118.64	112.60
1	D	165	GLN	CB-CG-CD	6.02	122.84	112.60
1	B	94	ARG	CD-NE-CZ	6.00	132.80	124.40
1	F	94	ARG	NE-CZ-NH1	5.99	127.49	121.50
2	O	497	ASN	CA-C-O	5.96	123.73	119.32
2	Q	441	THR	N-CA-CB	-5.96	102.05	110.51
2	O	450	ARG	CD-NE-CZ	-5.91	116.12	124.40
2	O	440	ARG	CB-CG-CD	-5.90	97.72	111.30
2	P	411	LYS	CB-CA-C	-5.90	100.94	110.74
2	P	383	ARG	CD-NE-CZ	-5.89	116.16	124.40
2	M	447	HIS	O-C-N	5.89	126.43	121.84
1	D	84	ASN	CA-CB-CG	5.89	118.49	112.60
2	Q	497	ASN	CA-C-N	5.89	125.76	119.28
2	Q	497	ASN	C-N-CA	5.89	125.76	119.28
2	M	514	ASN	O-C-N	5.88	127.83	121.12
1	B	52	LEU	CB-CA-C	5.88	122.47	109.94
1	F	61	HIS	CA-CB-CG	-5.88	107.92	113.80
1	C	158	LEU	CB-CA-C	5.87	120.53	110.79
1	A	37	ASN	N-CA-C	5.85	119.48	112.93
2	N	458	PRO	CB-CA-C	-5.84	103.58	111.12
2	N	533	THR	CA-CB-OG1	-5.84	100.84	109.60
2	P	351	PHE	CA-CB-CG	5.84	119.64	113.80
2	M	450	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	C	32	ASP	O-C-N	5.84	128.16	122.09
2	N	440	ARG	CB-CG-CD	-5.83	97.88	111.30
2	R	322	PRO	N-CA-C	5.83	122.27	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLU	CB-CG-CD	5.83	122.52	112.60
2	M	517	ASP	CA-CB-CG	5.82	118.42	112.60
2	R	447	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	94	ARG	NE-CZ-NH1	5.80	127.30	121.50
2	P	434	ASP	CA-CB-CG	-5.78	106.82	112.60
2	P	481	GLU	CB-CG-CD	5.78	122.42	112.60
2	R	496	ALA	N-CA-C	5.77	117.37	111.14
1	C	135	ILE	CB-CA-C	5.76	119.20	111.19
1	A	30	THR	CA-CB-OG1	-5.74	100.98	109.60
2	P	428	ARG	NE-CZ-NH2	-5.74	114.03	119.20
2	P	314	ASN	N-CA-C	-5.74	106.32	113.38
2	O	311	ARG	O-C-N	5.73	129.63	122.86
1	A	177	VAL	O-C-N	5.72	128.58	123.03
1	B	5	LEU	N-CA-C	-5.72	102.19	110.08
2	R	401	GLN	CB-CG-CD	5.70	122.29	112.60
1	C	150	GLN	N-CA-CB	5.69	118.26	110.01
2	R	494	SER	N-CA-C	-5.69	105.43	112.38
1	D	178	ASP	CA-CB-CG	-5.68	106.92	112.60
2	N	333	ARG	N-CA-C	-5.68	106.51	113.50
2	P	428	ARG	CB-CG-CD	5.68	124.35	111.30
1	E	52	LEU	CB-CA-C	5.67	122.03	109.94
1	C	5	LEU	O-C-N	5.67	127.76	121.53
1	E	171	ILE	N-CA-CB	-5.66	104.54	111.00
2	M	377	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	F	125	HIS	CA-CB-CG	-5.66	108.14	113.80
1	E	133	ARG	N-CA-C	-5.65	102.03	110.23
2	M	494	SER	N-CA-C	-5.65	105.49	112.38
2	M	410	HIS	CA-C-N	5.64	129.28	120.82
2	M	410	HIS	C-N-CA	5.64	129.28	120.82
2	O	496	ALA	N-CA-C	5.64	117.50	111.36
1	F	166	ARG	NE-CZ-NH1	5.64	127.14	121.50
2	N	361	HIS	CA-CB-CG	-5.62	108.18	113.80
2	Q	492	VAL	N-CA-C	-5.58	105.06	110.42
1	E	94	ARG	CD-NE-CZ	5.58	132.21	124.40
2	Q	515	PRO	CB-CA-C	5.57	118.64	111.56
2	M	377	ARG	NE-CZ-NH1	-5.57	115.94	121.50
2	M	314	ASN	CB-CA-C	5.56	119.41	109.29
1	C	129	SER	CA-C-N	5.56	130.67	123.00
1	C	129	SER	C-N-CA	5.56	130.67	123.00
1	B	136	ASN	OD1-CG-ND2	5.55	128.15	122.60
2	R	341	GLN	OE1-CD-NE2	-5.55	117.05	122.60
2	Q	533	THR	CA-CB-OG1	-5.54	101.29	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	110	LYS	O-C-N	5.54	126.13	121.31
1	C	171	ILE	N-CA-C	5.53	116.06	107.99
1	C	152	ASN	CA-CB-CG	5.52	118.12	112.60
2	P	380	VAL	N-CA-C	-5.52	99.69	107.75
2	Q	348	GLY	O-C-N	5.52	127.29	121.77
1	F	99	PHE	N-CA-C	-5.52	105.27	111.28
2	M	440	ARG	NH1-CZ-NH2	5.51	126.47	119.30
1	E	113	VAL	N-CA-CB	-5.51	102.71	110.26
1	E	7	GLU	CB-CG-CD	5.50	121.96	112.60
2	M	390	LYS	CA-CB-CG	5.50	125.09	114.10
2	R	339	ILE	O-C-N	5.50	125.15	121.69
2	N	387	GLN	CB-CG-CD	-5.50	103.26	112.60
1	C	47	GLU	CB-CA-C	-5.49	101.77	111.05
2	M	333	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	E	183	TYR	CA-CB-CG	5.47	123.74	113.90
2	O	440	ARG	CA-C-O	-5.47	114.45	120.36
1	D	57	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	23	LEU	CB-CA-C	5.45	119.88	110.84
1	A	77	GLY	N-CA-C	-5.44	106.15	115.08
2	P	489	CYS	N-CA-C	5.44	117.47	109.42
1	E	57	ASP	CA-C-N	5.43	126.93	120.14
1	E	57	ASP	C-N-CA	5.43	126.93	120.14
1	A	163	GLN	N-CA-C	5.43	117.30	109.04
2	N	454	ASN	CA-C-O	-5.43	115.69	121.78
2	O	385	VAL	CA-C-O	-5.43	116.14	121.67
2	Q	331	SER	O-C-N	5.42	126.59	121.38
1	A	133	ARG	N-CA-C	-5.42	102.25	110.28
2	R	358	ALA	O-C-N	5.42	127.86	122.12
1	D	177	VAL	O-C-N	5.41	128.28	123.03
2	Q	513	ALA	O-C-N	5.41	128.95	122.79
1	B	4	LEU	N-CA-CB	-5.40	102.23	110.49
2	R	474	LEU	N-CA-CB	-5.40	101.36	111.13
2	Q	465	ILE	O-C-N	5.39	129.03	123.20
1	A	94	ARG	NE-CZ-NH2	-5.39	114.35	119.20
2	R	440	ARG	CB-CG-CD	-5.39	98.91	111.30
1	B	94	ARG	NE-CZ-NH2	-5.38	114.35	119.20
1	E	94	ARG	NE-CZ-NH1	5.38	126.88	121.50
2	O	432	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	150	GLN	OE1-CD-NE2	5.38	127.98	122.60
2	P	457	ARG	N-CA-C	-5.37	103.27	109.93
2	R	333	ARG	N-CA-C	-5.37	106.90	113.50
2	Q	304	ASP	CA-CB-CG	-5.37	107.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	498	PRO	CB-CA-C	5.36	119.51	111.68
2	M	415	TYR	CB-CA-C	5.36	118.33	109.70
2	N	321	THR	CA-C-O	5.36	127.06	121.00
1	B	133	ARG	N-CA-C	-5.36	102.46	110.23
1	F	37	ASN	N-CA-C	5.36	118.93	112.93
2	R	458	PRO	CB-CA-C	-5.35	103.16	111.40
2	N	483	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	133	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	N	528	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	F	52	LEU	CB-CA-C	5.30	121.85	110.45
1	F	141	THR	CA-CB-CG2	5.30	119.52	110.50
1	F	184	ARG	CD-NE-CZ	-5.30	116.98	124.40
2	O	311	ARG	N-CA-CB	5.30	117.80	110.17
1	F	88	ALA	N-CA-C	-5.29	106.32	112.89
1	C	155	CYS	O-C-N	5.29	126.57	121.28
1	B	99	PHE	O-C-N	5.28	127.51	122.07
1	F	158	LEU	CB-CA-C	5.28	120.39	110.63
2	N	316	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	11	GLN	O-C-N	5.27	129.38	123.27
2	O	514	ASN	O-C-N	5.26	126.14	121.19
2	N	383	ARG	N-CA-CB	-5.25	101.50	111.00
1	D	122	MET	CA-C-O	-5.25	115.09	121.28
2	R	451	ASN	CA-C-N	-5.25	113.86	121.42
2	R	451	ASN	C-N-CA	-5.25	113.86	121.42
2	O	353	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	F	133	ARG	N-CA-C	-5.24	102.63	110.23
2	N	428	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	F	44	ALA	N-CA-C	-5.23	103.07	110.29
2	Q	451	ASN	N-CA-C	-5.23	100.14	108.30
2	N	479	TYR	CA-C-O	-5.22	115.35	121.46
2	Q	482	GLY	CA-C-O	-5.22	113.50	119.04
2	R	313	ARG	CB-CA-C	5.22	120.03	110.11
2	R	420	ASP	CB-CA-C	5.22	116.16	110.15
1	A	28	ASN	O-C-N	5.22	126.63	121.57
2	M	467	GLY	CA-C-N	5.22	124.83	119.56
2	M	467	GLY	C-N-CA	5.22	124.83	119.56
2	N	447	HIS	CB-CA-C	5.22	117.02	109.45
1	C	23	LEU	CB-CA-C	5.22	119.22	110.92
2	M	326	THR	CA-CB-OG1	-5.21	101.78	109.60
2	P	459	ALA	N-CA-C	-5.21	102.67	110.23
2	P	447	HIS	CA-CB-CG	-5.21	108.59	113.80
2	O	494	SER	N-CA-C	-5.21	106.19	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	ARG	CA-CB-CG	5.21	124.51	114.10
2	O	416	LEU	CB-CA-C	5.19	121.58	110.21
2	M	460	HIS	CA-CB-CG	-5.19	108.61	113.80
2	M	339	ILE	O-C-N	5.19	127.01	121.10
2	P	451	ASN	CA-C-O	-5.19	116.81	119.77
1	A	167	ARG	CD-NE-CZ	-5.18	117.14	124.40
2	O	305	ASN	CA-CB-CG	-5.18	107.42	112.60
2	M	385	VAL	O-C-N	5.18	128.70	123.00
1	E	3	GLU	CB-CG-CD	5.18	121.40	112.60
2	R	497	ASN	CA-C-O	5.18	123.15	119.32
1	F	100	ASP	O-C-N	5.17	127.40	122.07
1	B	106	LEU	CA-CB-CG	5.17	134.40	116.30
2	R	468	PRO	N-CA-C	5.17	120.32	113.86
2	N	471	ALA	N-CA-CB	5.16	118.28	110.28
2	R	323	ASP	O-C-N	5.16	128.62	122.27
2	O	385	VAL	O-C-N	5.15	128.67	123.00
2	P	326	THR	CA-CB-OG1	-5.15	101.88	109.60
2	Q	450	ARG	CA-C-O	-5.14	116.19	122.41
2	R	458	PRO	N-CA-C	-5.14	103.98	111.33
2	O	333	ARG	CB-CA-C	5.14	119.98	109.55
1	E	165	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	178	ASP	CA-CB-CG	-5.13	107.47	112.60
2	P	365	LEU	N-CA-C	5.13	120.54	113.97
1	F	39	LEU	O-C-N	5.13	128.00	122.15
1	B	171	ILE	N-CA-C	5.12	115.14	107.51
1	E	103	GLU	CA-C-O	-5.12	115.17	120.70
1	F	114	VAL	CA-C-O	-5.12	116.30	121.67
1	A	169	THR	CA-CB-CG2	5.12	119.20	110.50
1	F	46	GLY	CA-C-O	-5.11	118.77	122.45
2	O	315	TRP	CA-C-O	5.11	126.69	120.31
1	A	155	CYS	O-C-N	5.11	125.84	121.30
2	P	451	ASN	N-CA-C	-5.10	100.34	108.30
2	P	494	SER	N-CA-C	-5.10	106.89	113.01
1	E	4	LEU	CA-C-O	-5.10	115.64	121.82
2	Q	359	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	38	ARG	NE-CZ-NH2	-5.10	114.61	119.20
2	Q	403	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	F	36	TRP	N-CA-C	5.09	118.07	108.65
2	R	451	ASN	N-CA-C	-5.09	99.95	110.80
2	P	497	ASN	CA-C-N	5.09	124.88	119.28
2	P	497	ASN	C-N-CA	5.09	124.88	119.28
2	R	359	HIS	CA-CB-CG	-5.09	108.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	N-CA-C	-5.09	100.61	108.90
2	Q	428	ARG	CG-CD-NE	5.09	123.19	112.00
2	Q	458	PRO	N-CA-C	-5.09	103.78	111.41
2	N	450	ARG	CA-C-O	-5.08	116.26	122.41
2	O	442	ILE	CB-CA-C	5.08	118.65	110.82
1	F	103	GLU	CG-CD-OE1	-5.08	106.72	118.40
1	A	196	VAL	O-C-N	5.08	128.14	122.61
2	Q	504	LEU	CA-C-N	-5.08	116.03	122.37
2	Q	504	LEU	C-N-CA	-5.08	116.03	122.37
1	F	106	LEU	CA-CB-CG	5.08	134.06	116.30
2	R	420	ASP	CA-CB-CG	5.07	117.67	112.60
2	O	450	ARG	CA-C-O	-5.07	115.73	121.66
2	O	316	HIS	CA-CB-CG	-5.06	108.74	113.80
2	O	440	ARG	NH1-CZ-NH2	5.05	125.87	119.30
1	A	52	LEU	CB-CA-C	5.04	120.67	109.94
2	P	457	ARG	CD-NE-CZ	5.04	131.45	124.40
2	P	392	VAL	O-C-N	5.03	126.83	121.10
2	N	320	LEU	CA-C-O	-5.02	115.32	120.54
1	E	47	GLU	CA-CB-CG	5.02	124.14	114.10
2	P	341	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	136	ASN	O-C-N	5.01	127.86	122.15
2	Q	311	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	ARG	Sidechain
2	P	440	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	31	0
1	B	1571	0	1499	31	0
1	C	1571	0	1499	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1571	0	1499	26	0
1	E	1571	0	1499	47	0
1	F	1571	0	1499	47	0
2	M	1838	0	1791	48	0
2	N	1838	0	1791	22	0
2	O	1838	0	1791	32	0
2	P	1838	0	1791	45	0
2	Q	1838	0	1791	40	0
2	R	1838	0	1791	39	0
3	M	4	0	0	1	0
3	N	4	0	0	0	0
3	O	4	0	0	0	0
3	P	4	0	0	1	0
3	Q	4	0	0	0	0
3	R	4	0	0	1	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	M	4	0	5	0	0
5	N	4	0	5	0	0
5	O	4	0	5	1	0
5	P	4	0	5	0	0
5	Q	4	0	5	2	0
5	R	4	0	5	0	0
6	A	73	0	0	0	0
6	B	79	0	0	0	0
6	C	78	0	0	0	0
6	D	81	0	0	0	0
6	E	82	0	0	1	0
6	F	80	0	0	0	0
6	M	161	0	0	4	0
6	N	163	0	0	3	0
6	O	156	0	0	3	0
6	P	151	0	0	3	0
6	Q	159	0	0	2	0
6	R	159	0	0	2	0
All	All	21930	0	19770	411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (411) 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:F:165:GLN:H	1:F:165:GLN:HE21	0.97	0.93
1:E:165:GLN:H	1:E:165:GLN:NE2	1.64	0.93
1:F:165:GLN:H	1:F:165:GLN:NE2	1.66	0.93
1:E:165:GLN:H	1:E:165:GLN:HE21	1.05	0.92
2:M:497:ASN:HD22	2:M:499:GLU:H	1.22	0.87
1:C:165:GLN:H	1:C:165:GLN:NE2	1.73	0.86
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.58	0.85
2:R:361:HIS:H	2:R:361:HIS:CD2	1.90	0.84
1:A:165:GLN:H	1:A:165:GLN:HE21	1.27	0.83
2:R:505:ILE:O	2:R:507:LYS:HE3	1.79	0.82
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.61	0.81
2:O:361:HIS:H	2:O:361:HIS:CD2	1.99	0.81
2:R:361:HIS:H	2:R:361:HIS:HD2	1.28	0.80
1:E:70:VAL:HG11	1:E:106:LEU:HD21	1.64	0.80
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.64	0.79
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.18	0.79
1:B:176:GLU:HG3	1:B:180:LYS:C	2.08	0.79
1:B:176:GLU:HG3	1:B:180:LYS:O	1.84	0.78
1:A:165:GLN:H	1:A:165:GLN:NE2	1.82	0.78
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.49	0.78
1:B:165:GLN:H	1:B:165:GLN:HE21	1.33	0.76
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.00	0.76
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.67	0.76
1:C:165:GLN:H	1:C:165:GLN:HE21	1.32	0.75
2:M:522:ARG:NH1	6:M:669:HOH:O	2.17	0.75
3:M:550:CO3:O1	6:M:727:HOH:O	2.05	0.75
2:O:413:ASP:C	2:O:414:ARG:HD2	2.13	0.73
2:N:390:LYS:HE2	6:N:732:HOH:O	1.88	0.73
2:M:361:HIS:H	2:M:361:HIS:CD2	2.04	0.73
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.87	0.73
1:C:44:ALA:O	1:C:48:HIS:NE2	2.19	0.72
1:E:165:GLN:HE21	1:E:165:GLN:N	1.86	0.72
1:B:165:GLN:H	1:B:165:GLN:NE2	1.88	0.72
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.26	0.71
2:P:361:HIS:H	2:P:361:HIS:CD2	2.08	0.71
1:A:176:GLU:HG3	1:A:180:LYS:O	1.91	0.71
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.06	0.70
2:O:361:HIS:H	2:O:361:HIS:HD2	1.39	0.70
2:M:497:ASN:ND2	2:M:499:GLU:H	1.89	0.70
2:R:447:HIS:NE2	3:R:550:CO3:O2	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:361:HIS:H	2:M:361:HIS:HD2	1.40	0.69
1:D:165:GLN:NE2	1:D:165:GLN:H	1.89	0.69
2:R:361:HIS:CD2	2:R:361:HIS:N	2.61	0.69
1:F:165:GLN:HE21	1:F:165:GLN:N	1.81	0.69
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.10	0.68
2:R:497:ASN:ND2	2:R:499:GLU:H	1.91	0.68
1:F:50:LEU:HD12	1:F:51:LEU:N	2.09	0.67
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.75	0.67
1:A:176:GLU:HA	1:A:180:LYS:O	1.94	0.67
2:Q:390:LYS:HD2	6:Q:1025:HOH:O	1.92	0.67
2:O:390:LYS:HD2	6:O:648:HOH:O	1.95	0.67
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.95	0.66
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.59	0.66
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.92	0.66
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.60	0.66
2:O:416:LEU:C	2:O:416:LEU:HD23	2.20	0.66
1:F:70:VAL:HG11	1:F:106:LEU:HD21	1.78	0.66
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.60	0.65
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	1.95	0.64
1:C:3:GLU:OE1	1:C:3:GLU:HA	1.97	0.64
1:F:147:ASP:OD2	1:F:174:ARG:HD2	1.97	0.64
2:N:497:ASN:HD22	2:N:499:GLU:H	1.45	0.64
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.63	0.64
2:P:478:LEU:C	2:P:478:LEU:HD23	2.23	0.63
2:P:361:HIS:H	2:P:361:HIS:HD2	1.44	0.63
2:R:413:ASP:C	2:R:414:ARG:HD2	2.23	0.63
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.34	0.63
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.61	0.63
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.78	0.62
1:A:78:GLU:CG	2:M:301:PRO:HB3	2.29	0.62
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.99	0.62
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.14	0.62
1:B:70:VAL:HG11	1:B:106:LEU:HD21	1.81	0.62
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.00	0.62
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.65	0.61
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.82	0.61
2:P:414:ARG:NE	2:P:414:ARG:HA	2.16	0.60
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.27	0.60
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.82	0.60
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.37	0.60
2:R:497:ASN:HD22	2:R:499:GLU:H	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.66	0.59
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.37	0.59
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.36	0.59
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.17	0.59
1:A:180:LYS:HG2	1:A:181:THR:N	2.17	0.59
2:N:390:LYS:HD3	6:N:651:HOH:O	2.02	0.59
2:P:356:PHE:HD2	2:P:428:ARG:HD3	1.67	0.59
2:O:497:ASN:HD22	2:O:499:GLU:H	1.50	0.59
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.37	0.59
2:R:473:LYS:NZ	6:R:1368:HOH:O	2.36	0.59
2:O:447:HIS:HB2	2:O:448:PRO:HD2	1.84	0.58
1:D:165:GLN:H	1:D:165:GLN:HE21	1.50	0.58
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.33	0.58
1:A:78:GLU:CG	2:M:301:PRO:CB	2.82	0.58
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.51	0.58
2:Q:390:LYS:HD3	6:Q:1146:HOH:O	2.04	0.58
2:Q:361:HIS:CG	5:Q:601:BME:H21	2.39	0.58
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.86	0.58
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.39	0.58
1:D:110:LYS:NZ	1:D:147:ASP:OD1	2.36	0.57
1:D:114:VAL:HG23	1:D:122:MET:HE3	1.86	0.57
2:O:320:LEU:HG	2:O:322:PRO:HD3	1.87	0.57
1:C:165:GLN:HE21	1:C:165:GLN:N	2.02	0.57
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.05	0.57
2:Q:438:SER:O	5:Q:601:BME:H22	2.05	0.57
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.34	0.57
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.40	0.57
2:N:361:HIS:CD2	2:N:361:HIS:H	2.23	0.56
2:O:399:MET:HA	2:O:462:HIS:O	2.05	0.56
2:P:416:LEU:C	2:P:416:LEU:HD23	2.30	0.56
1:F:177:VAL:O	1:F:180:LYS:HB3	2.05	0.56
2:R:447:HIS:HB2	2:R:448:PRO:HD2	1.87	0.56
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.05	0.56
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.86	0.56
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.87	0.56
1:C:177:VAL:O	1:C:180:LYS:HB3	2.06	0.56
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.88	0.55
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.54	0.55
1:C:36:TRP:CG	1:C:37:ASN:H	2.24	0.55
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.40	0.55
2:O:497:ASN:ND2	2:O:499:GLU:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:GLN:HG3	1:F:184:ARG:HH22	1.72	0.55
1:A:78:GLU:HG3	2:M:301:PRO:CB	2.36	0.55
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.42	0.55
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.42	0.55
1:C:143:LEU:HD23	1:C:143:LEU:C	2.32	0.55
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.21	0.55
2:P:335:ALA:HB2	2:R:328:ILE:HD12	1.89	0.54
1:D:180:LYS:HG3	1:D:181:THR:N	2.22	0.54
2:P:362:ASP:OD1	2:P:440:ARG:HD2	2.08	0.54
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.88	0.54
1:F:36:TRP:CG	1:F:37:ASN:H	2.25	0.54
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.90	0.54
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.15	0.54
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.33	0.54
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.54
2:R:497:ASN:HD22	2:R:498:PRO:N	2.05	0.53
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.56	0.53
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.38	0.53
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.89	0.53
2:M:450:ARG:HG3	6:M:635:HOH:O	2.08	0.53
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.24	0.53
1:F:176:GLU:HG3	1:F:180:LYS:N	2.23	0.53
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.55	0.53
2:M:416:LEU:C	2:M:416:LEU:CD2	2.81	0.53
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.24	0.53
1:A:114:VAL:HG23	1:A:122:MET:CE	2.37	0.53
1:B:144:TYR:CE1	1:B:158:LEU:HD13	2.44	0.53
1:F:176:GLU:OE2	1:F:179:GLY:C	2.52	0.53
2:P:356:PHE:CD2	2:P:428:ARG:HD3	2.43	0.52
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.09	0.52
2:R:316:HIS:HB3	2:R:317:PRO:HD2	1.92	0.52
2:R:473:LYS:HD2	2:R:474:LEU:N	2.25	0.52
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.24	0.52
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.08	0.52
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.74	0.52
2:R:497:ASN:HD22	2:R:497:ASN:C	2.18	0.52
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.72	0.52
2:R:416:LEU:C	2:R:416:LEU:HD23	2.34	0.52
2:P:414:ARG:HD2	2:P:414:ARG:N	2.24	0.52
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.58	0.52
2:R:390:LYS:HE2	6:R:1383:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:478:LEU:C	2:R:478:LEU:HD23	2.35	0.52
2:N:414:ARG:NE	2:N:414:ARG:HA	2.26	0.52
2:P:383:ARG:NE	2:P:434:ASP:O	2.37	0.51
1:E:144:TYR:CE1	1:E:158:LEU:HD13	2.44	0.51
1:F:144:TYR:CE1	1:F:158:LEU:HD13	2.46	0.51
2:N:478:LEU:C	2:N:478:LEU:HD23	2.35	0.51
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.92	0.51
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.93	0.51
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.92	0.51
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.51
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.92	0.51
1:E:176:GLU:HG3	1:E:180:LYS:O	2.11	0.51
2:M:478:LEU:HD23	2:M:478:LEU:C	2.35	0.51
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.11	0.51
1:A:143:LEU:C	1:A:143:LEU:HD23	2.35	0.51
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.46	0.51
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.93	0.51
1:F:50:LEU:O	1:F:182:ALA:HA	2.11	0.51
2:N:497:ASN:ND2	2:N:499:GLU:H	2.09	0.50
1:E:58:GLY:HA2	1:E:190:GLN:HB3	1.93	0.50
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.11	0.50
2:O:416:LEU:C	2:O:416:LEU:CD2	2.84	0.50
2:O:413:ASP:O	2:O:414:ARG:HD2	2.11	0.50
2:N:473:LYS:NZ	6:N:723:HOH:O	2.35	0.50
1:D:51:LEU:O	1:D:105:THR:HA	2.11	0.50
2:M:488:MET:HE1	2:P:508:LEU:HD23	1.94	0.50
1:A:41:LYS:O	1:A:48:HIS:HE1	1.95	0.50
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.47	0.50
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.27	0.50
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.09	0.50
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.47	0.50
2:Q:363:LEU:N	2:Q:363:LEU:HD12	2.27	0.50
1:F:190:GLN:HG3	2:R:333:ARG:HG2	1.93	0.49
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.94	0.49
1:F:176:GLU:HA	1:F:180:LYS:O	2.12	0.49
1:C:131:PHE:O	1:C:132:ALA:HB2	2.12	0.49
1:D:36:TRP:CG	1:D:37:ASN:H	2.30	0.49
2:O:361:HIS:CD2	2:O:361:HIS:N	2.71	0.49
2:O:414:ARG:HD2	2:O:414:ARG:N	2.26	0.49
1:E:176:GLU:HG2	1:E:179:GLY:C	2.38	0.49
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:497:ASN:C	2:P:497:ASN:HD22	2.21	0.49
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.95	0.49
1:F:52:LEU:C	1:F:52:LEU:HD22	2.37	0.49
1:F:180:LYS:HD2	1:F:181:THR:N	2.27	0.49
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.95	0.49
1:F:143:LEU:C	1:F:143:LEU:HD23	2.37	0.49
1:A:50:LEU:O	1:A:182:ALA:HA	2.13	0.49
1:B:176:GLU:OE2	1:B:179:GLY:C	2.55	0.48
2:O:473:LYS:NZ	6:O:722:HOH:O	2.32	0.48
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.93	0.48
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.43	0.48
1:B:52:LEU:C	1:B:52:LEU:HD22	2.38	0.48
1:C:52:LEU:HD21	1:C:184:ARG:HH11	1.79	0.48
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.29	0.48
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.95	0.48
2:O:522:ARG:NH1	6:O:673:HOH:O	2.17	0.48
1:E:6:PRO:HB2	2:Q:503:GLN:HE22	1.78	0.48
1:C:52:LEU:C	1:C:52:LEU:HD22	2.38	0.48
1:F:110:LYS:HE2	1:F:148:GLU:OE2	2.13	0.48
1:B:176:GLU:OE2	1:B:179:GLY:O	2.31	0.48
1:D:177:VAL:O	1:D:180:LYS:HB3	2.14	0.48
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.96	0.47
2:P:416:LEU:C	2:P:416:LEU:CD2	2.87	0.47
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.77	0.47
1:F:114:VAL:HG23	1:F:122:MET:HE3	1.95	0.47
2:M:442:ILE:HD12	2:M:442:ILE:O	2.14	0.47
2:P:390:LYS:HD2	6:P:648:HOH:O	2.13	0.47
1:E:133:ARG:HG3	2:Q:326:THR:HG21	1.96	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.66	0.47
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.15	0.47
2:P:411:LYS:O	2:P:414:ARG:NH1	2.44	0.47
2:P:516:MET:HB3	2:P:516:MET:HE3	1.66	0.47
1:E:176:GLU:HA	1:E:180:LYS:O	2.15	0.47
1:C:3:GLU:OE1	1:C:3:GLU:CA	2.63	0.47
2:Q:522:ARG:NE	2:Q:524:ASP:OD1	2.47	0.47
1:C:24:GLU:O	1:C:27:GLY:N	2.44	0.47
1:E:36:TRP:CG	1:E:37:ASN:H	2.33	0.47
2:Q:399:MET:HA	2:Q:462:HIS:O	2.14	0.47
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.97	0.47
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.63	0.46
1:D:163:GLN:HB3	1:D:165:GLN:HE21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	1.97	0.46
2:P:447:HIS:HB2	2:P:448:PRO:HD2	1.97	0.46
2:P:376:GLU:O	2:P:442:ILE:HA	2.15	0.46
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.30	0.46
1:F:103:GLU:OE2	1:F:184:ARG:NH1	2.35	0.46
2:R:385:VAL:O	2:R:526:VAL:HA	2.15	0.46
2:M:356:PHE:CE1	2:M:428:ARG:HD3	2.50	0.46
1:C:63:VAL:HG12	1:C:66:SER:HB3	1.97	0.46
1:B:176:GLU:HA	1:B:180:LYS:O	2.16	0.46
2:O:362:ASP:OD1	2:O:440:ARG:HD3	2.16	0.46
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.98	0.46
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.83	0.46
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.39	0.46
2:P:437:TYR:CD1	2:P:437:TYR:C	2.94	0.46
2:R:400:TRP:HA	2:R:425:GLY:O	2.16	0.46
1:D:52:LEU:C	1:D:52:LEU:HD22	2.42	0.45
1:E:44:ALA:HB2	1:E:88:ALA:O	2.16	0.45
1:F:115:ASN:HA	1:F:121:PRO:HA	1.98	0.45
1:A:176:GLU:HG2	1:A:179:GLY:HA2	1.97	0.45
2:P:326:THR:HG22	2:P:330:ARG:HD2	1.97	0.45
1:E:177:VAL:O	1:E:180:LYS:HB3	2.17	0.45
1:C:31:ARG:HH12	2:O:428:ARG:HG2	1.81	0.45
2:P:447:HIS:CG	6:P:654:HOH:O	2.69	0.45
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.85	0.45
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.98	0.45
1:E:28:ASN:HB3	6:E:271:HOH:O	2.16	0.45
2:M:390:LYS:HE2	6:M:726:HOH:O	2.16	0.45
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.16	0.45
1:E:24:GLU:O	1:E:27:GLY:N	2.35	0.45
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.40	0.45
1:B:19:ILE:O	2:N:426:VAL:HG21	2.17	0.45
2:P:359:HIS:O	2:P:366:ASN:HB3	2.17	0.45
2:M:497:ASN:HD22	2:M:499:GLU:N	2.02	0.45
1:B:36:TRP:CG	1:B:37:ASN:H	2.34	0.45
1:E:58:GLY:CA	1:E:190:GLN:HB3	2.46	0.45
1:A:36:TRP:CG	1:A:37:ASN:H	2.34	0.45
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.98	0.45
2:Q:522:ARG:HE	2:Q:524:ASP:CG	2.25	0.45
1:A:176:GLU:HG3	1:A:180:LYS:N	2.31	0.44
2:R:414:ARG:HD2	2:R:414:ARG:N	2.32	0.44
1:B:12:THR:HA	1:B:135:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLU:HG3	1:C:180:LYS:O	2.18	0.44
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.81	0.44
2:R:516:MET:HE3	2:R:516:MET:HB3	1.78	0.44
1:B:176:GLU:HG2	1:B:179:GLY:HA2	2.00	0.44
2:M:376:GLU:O	2:M:442:ILE:HA	2.17	0.44
2:N:414:ARG:NE	2:N:414:ARG:CA	2.78	0.44
1:D:143:LEU:C	1:D:143:LEU:HD23	2.43	0.44
1:E:174:ARG:HH21	1:E:181:THR:HG21	1.82	0.44
1:B:4:LEU:HD22	2:P:511:ASN:CG	2.43	0.44
2:P:399:MET:HA	2:P:462:HIS:O	2.17	0.44
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.84	0.44
1:F:54:GLN:HG3	1:F:103:GLU:HG3	2.00	0.44
1:B:176:GLU:HG2	1:B:179:GLY:C	2.43	0.44
2:P:447:HIS:NE2	3:P:550:CO3:O2	2.42	0.44
2:P:536:GLU:HB2	6:P:705:HOH:O	2.18	0.44
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.18	0.44
2:Q:434:ASP:HB3	2:Q:436:TYR:CD2	2.53	0.44
2:N:362:ASP:OD1	2:N:440:ARG:HD3	2.18	0.43
2:Q:437:TYR:CD1	2:Q:437:TYR:C	2.96	0.43
1:C:79:TYR:O	2:O:301:PRO:HB2	2.18	0.43
2:R:386:ASP:HA	2:R:527:LEU:O	2.18	0.43
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.85	0.43
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.79	0.43
1:E:174:ARG:HH21	1:E:181:THR:CG2	2.32	0.43
1:F:50:LEU:HD12	1:F:50:LEU:C	2.42	0.43
1:F:133:ARG:HG3	2:R:326:THR:HG21	2.00	0.43
2:R:359:HIS:O	2:R:366:ASN:HB3	2.18	0.43
2:M:377:ARG:HH11	2:M:377:ARG:HD2	1.52	0.43
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.52	0.43
2:Q:356:PHE:HD2	2:Q:428:ARG:HD3	1.83	0.43
1:C:50:LEU:O	1:C:182:ALA:HA	2.18	0.43
2:O:376:GLU:O	2:O:442:ILE:HA	2.19	0.43
1:D:50:LEU:HD12	1:D:51:LEU:N	2.33	0.43
1:E:188:ARG:NH1	1:E:188:ARG:HG3	2.34	0.43
2:M:442:ILE:HD12	2:M:442:ILE:C	2.44	0.43
1:B:143:LEU:C	1:B:143:LEU:HD23	2.44	0.43
2:P:361:HIS:CD2	2:P:361:HIS:N	2.79	0.43
2:O:450:ARG:HH11	2:O:450:ARG:HD2	1.60	0.43
2:P:453:PRO:HG2	2:Q:310:ILE:HG23	2.01	0.43
1:B:165:GLN:HE21	1:B:165:GLN:N	2.09	0.43
2:N:359:HIS:O	2:N:366:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:361:HIS:CG	5:O:601:BME:H21	2.54	0.43
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.75	0.43
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.44	0.43
1:B:114:VAL:HG23	1:B:122:MET:CE	2.49	0.43
2:P:407:ARG:HD3	2:P:417:ALA:O	2.18	0.43
1:E:143:LEU:HD23	1:E:143:LEU:C	2.44	0.43
1:E:163:GLN:HA	1:E:164:PRO:HD3	1.80	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.01	0.43
2:R:373:PRO:HB3	2:R:423:PHE:HB2	2.01	0.43
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.72	0.42
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.18	0.42
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.53	0.42
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.48	0.42
2:N:447:HIS:HB2	2:N:448:PRO:HD2	2.01	0.42
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.49	0.42
1:E:41:LYS:HZ2	1:E:86:GLU:C	2.27	0.42
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.43	0.42
1:F:52:LEU:HA	1:F:104:TRP:O	2.19	0.42
1:F:131:PHE:O	1:F:132:ALA:HB2	2.19	0.42
2:R:343:ILE:HG13	2:R:343:ILE:O	2.19	0.42
2:M:399:MET:HA	2:M:462:HIS:O	2.19	0.42
1:C:70:VAL:HG21	1:C:106:LEU:HD21	2.01	0.42
2:N:379:ILE:CD1	2:N:518:CYS:SG	3.07	0.42
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.00	0.42
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.66	0.42
2:M:328:ILE:HD12	2:N:335:ALA:HB2	2.00	0.42
1:E:41:LYS:O	1:E:42:PRO:C	2.63	0.42
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.81	0.42
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.87	0.42
2:O:359:HIS:O	2:O:366:ASN:HB3	2.19	0.42
1:D:50:LEU:O	1:D:182:ALA:HA	2.20	0.42
1:F:54:GLN:OE1	1:F:184:ARG:NH2	2.52	0.42
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.54	0.42
2:O:411:LYS:O	2:O:414:ARG:HD3	2.20	0.42
2:M:416:LEU:C	2:M:416:LEU:HD23	2.44	0.41
2:M:420:ASP:HA	2:M:421:PRO:HD2	1.79	0.41
2:M:451:ASN:HB3	2:M:455:ASP:OD2	2.20	0.41
2:P:335:ALA:HB1	2:R:325:LYS:HG2	2.00	0.41
1:E:5:LEU:HA	1:E:6:PRO:HD3	1.84	0.41
1:F:19:ILE:O	2:R:426:VAL:HG21	2.20	0.41
1:A:4:LEU:HB3	2:M:387:GLN:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.36	0.41
2:M:304:ASP:HB2	2:M:343:ILE:HG13	2.01	0.41
2:M:534:HIS:O	2:M:535:PHE:C	2.63	0.41
2:M:385:VAL:O	2:M:526:VAL:HA	2.19	0.41
1:B:57:ASP:OD1	1:B:57:ASP:C	2.63	0.41
1:B:68:LEU:HD12	1:B:68:LEU:N	2.36	0.41
2:N:361:HIS:H	2:N:361:HIS:HD2	1.66	0.41
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.85	0.41
1:D:24:GLU:O	1:D:27:GLY:N	2.40	0.41
2:Q:306:SER:OG	2:Q:530:GLN:NE2	2.44	0.41
1:A:176:GLU:HG3	1:A:180:LYS:C	2.43	0.41
1:B:35:ILE:HD13	2:N:351:PHE:CE1	2.55	0.41
1:B:114:VAL:CG2	1:B:122:MET:HE3	2.51	0.41
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.78	0.41
1:E:131:PHE:O	1:E:132:ALA:HB2	2.21	0.41
1:F:19:ILE:HD13	1:F:19:ILE:HG21	1.89	0.41
1:F:50:LEU:HD12	1:F:51:LEU:H	1.85	0.41
1:B:20:GLY:O	1:B:21:LEU:HD23	2.20	0.41
2:Q:414:ARG:HD2	2:Q:414:ARG:N	2.36	0.41
1:F:147:ASP:OD2	1:F:174:ARG:NH1	2.54	0.41
2:P:390:LYS:HA	2:P:391:PRO:HD3	1.96	0.41
1:A:78:GLU:HG3	2:M:301:PRO:HB2	2.03	0.41
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.99	0.41
2:P:497:ASN:O	2:P:500:ALA:HB3	2.21	0.41
2:R:437:TYR:CD1	2:R:437:TYR:C	2.98	0.41
1:A:133:ARG:HG3	2:M:326:THR:HG21	2.02	0.40
2:N:326:THR:HG22	2:N:330:ARG:HD2	2.02	0.40
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.21	0.40
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.56	0.40
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.94	0.40
2:P:486:ILE:HB	2:P:487:PRO:HD3	2.02	0.40
1:E:180:LYS:HD2	1:E:181:THR:O	2.21	0.40
1:E:199:ASP:CG	2:Q:313:ARG:HE	2.30	0.40
2:M:363:LEU:HD12	2:M:363:LEU:N	2.36	0.40
2:N:379:ILE:HD12	2:N:518:CYS:SG	2.61	0.40
2:N:399:MET:HA	2:N:462:HIS:O	2.20	0.40
1:D:77:GLY:O	1:D:114:VAL:HG12	2.22	0.40
2:P:497:ASN:HD22	2:P:499:GLU:H	1.70	0.40
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.22	0.40
2:R:363:LEU:N	2:R:363:LEU:HD12	2.37	0.40
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.84	0.40
1:F:36:TRP:CD1	1:F:37:ASN:H	2.39	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%)	190 (96%)	8 (4%)	0	100	100
1	B	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	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%)	224 (98%)	5 (2%)	0	100	100
All	All	2562/2628 (98%)	2482 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	155 (96%)	7 (4%)	26	27
1	B	162/163 (99%)	156 (96%)	6 (4%)	30	33
1	C	162/163 (99%)	154 (95%)	8 (5%)	22	22
1	D	162/163 (99%)	155 (96%)	7 (4%)	26	27
1	E	162/163 (99%)	154 (95%)	8 (5%)	22	22
1	F	162/163 (99%)	152 (94%)	10 (6%)	16	14
2	M	196/202 (97%)	185 (94%)	11 (6%)	19	18
2	N	196/202 (97%)	189 (96%)	7 (4%)	31	34
2	O	196/202 (97%)	188 (96%)	8 (4%)	27	29
2	P	196/202 (97%)	185 (94%)	11 (6%)	19	18
2	Q	196/202 (97%)	186 (95%)	10 (5%)	21	21
2	R	196/202 (97%)	187 (95%)	9 (5%)	24	25
All	All	2148/2190 (98%)	2046 (95%)	102 (5%)	23	24

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	38	ARG
1	A	43	ASP
1	A	47	GLU
1	A	52	LEU
1	A	143	LEU
1	A	165	GLN
2	M	301	PRO
2	M	343	ILE
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	433	SER
2	M	434	ASP

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Mol	Chain	Res	Type
2	M	478	LEU
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	32	ASP
1	B	52	LEU
1	B	143	LEU
1	B	165	GLN
1	B	180	LYS
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	416	LEU
2	N	478	LEU
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	126	ILE
1	C	154	LYS
1	C	165	GLN
1	C	192	GLU
2	O	364	LEU
2	O	372	LEU
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	52	LEU
1	D	106	LEU
1	D	143	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	372	LEU

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Mol	Chain	Res	Type
2	P	395	THR
2	P	414	ARG
2	P	416	LEU
2	P	433	SER
2	P	434	ASP
2	P	440	ARG
2	P	478	LEU
2	P	503	GLN
2	P	534	HIS
1	E	4	LEU
1	E	38	ARG
1	E	47	GLU
1	E	49	ILE
1	E	52	LEU
1	E	114	VAL
1	E	165	GLN
1	E	180	LYS
2	Q	352	SER
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	442	ILE
2	Q	478	LEU
2	Q	503	GLN
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	38	ARG
1	F	50	LEU
1	F	52	LEU
1	F	154	LYS
1	F	165	GLN
1	F	178	ASP
1	F	180	LYS
1	F	181	THR
2	R	343	ILE
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	434	ASP

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Mol	Chain	Res	Type
2	R	442	ILE
2	R	478	LEU
2	R	503	GLN
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	136	ASN
1	B	140	HIS
1	B	163	GLN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	87	ASN
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
1	D	136	ASN
1	D	163	GLN
1	D	165	GLN
2	P	334	GLN
2	P	361	HIS
2	P	394	ASN
2	P	412	ASN
2	P	497	ASN
2	P	514	ASN
1	E	163	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	394	ASN

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Mol	Chain	Res	Type
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
2	Q	534	HIS
1	F	59	ASN
1	F	115	ASN
1	F	163	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	422	ASN
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 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
3	CO3	R	550	4	3,3,3	1.71	1 (33%)	2,3,3	1.84	1 (50%)
3	CO3	Q	550	4	3,3,3	2.67	1 (33%)	2,3,3	3.31	2 (100%)
5	BME	P	601	2	3,3,3	0.40	0	2,2,2	0.93	0
3	CO3	N	550	4	3,3,3	1.53	1 (33%)	2,3,3	1.15	0
5	BME	O	601	2	3,3,3	0.35	0	2,2,2	0.83	0
5	BME	M	601	2	3,3,3	0.38	0	2,2,2	0.38	0
5	BME	R	601	2	3,3,3	0.27	0	2,2,2	0.09	0
3	CO3	P	550	4	3,3,3	1.76	1 (33%)	2,3,3	0.74	0
5	BME	Q	601	2	3,3,3	0.57	0	2,2,2	0.85	0
5	BME	N	601	2	3,3,3	0.27	0	2,2,2	0.39	0
3	CO3	M	550	4	3,3,3	1.53	1 (33%)	2,3,3	1.08	0
3	CO3	O	550	4	3,3,3	1.95	1 (33%)	2,3,3	1.50	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	BME	P	601	2	-	0/1/1/1	-
5	BME	O	601	2	-	0/1/1/1	-
5	BME	M	601	2	-	1/1/1/1	-
5	BME	R	601	2	-	0/1/1/1	-
5	BME	Q	601	2	-	0/1/1/1	-
5	BME	N	601	2	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	550	CO3	O1-C	4.47	1.41	1.25
3	O	550	CO3	O1-C	3.24	1.36	1.25
3	P	550	CO3	O1-C	2.97	1.36	1.25
3	R	550	CO3	O1-C	2.79	1.35	1.25
3	N	550	CO3	O1-C	2.60	1.34	1.25
3	M	550	CO3	O1-C	2.57	1.34	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	550	CO3	O3-C-O1	-3.76	110.06	119.68
3	Q	550	CO3	O2-C-O1	-2.79	112.54	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	550	CO3	O3-C-O1	-2.51	113.25	119.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	601	BME	O1-C1-C2-S2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	550	CO3	1	0
5	O	601	BME	1	0
3	P	550	CO3	1	0
5	Q	601	BME	2	0
3	M	550	CO3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.