



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:33 PM EDT

PDB ID : 3PCD
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.35.1

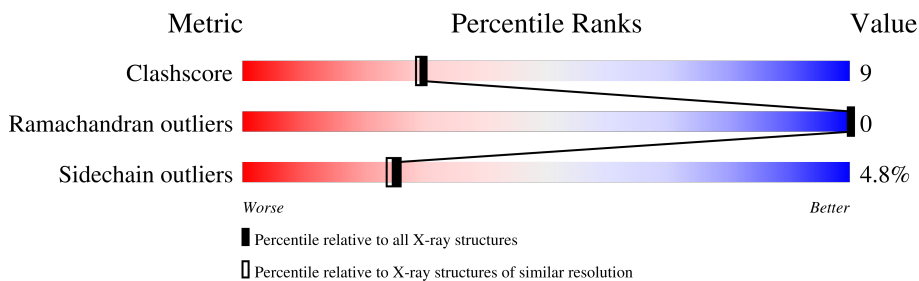
1 Overall quality at a glance

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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	80% (green), 15% (yellow), 5% (orange), 0% (red), 0% (grey)
1	B	200	78% (green), 18% (yellow), 4% (orange), 0% (red), 0% (grey)
1	C	200	77% (green), 18% (yellow), 5% (orange), 0% (red), 0% (grey)
1	D	200	78% (green), 18% (yellow), 4% (orange), 0% (red), 0% (grey)
1	E	200	72% (green), 23% (yellow), 5% (orange), 0% (red), 0% (grey)
1	F	200	72% (green), 22% (yellow), 6% (orange), 0% (red), 0% (grey)
2	M	238	73% (green), 21% (yellow), 6% (orange), 0% (red), 0% (grey)
2	N	238	78% (green), 17% (yellow), 5% (orange), 0% (red), 0% (grey)

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Mol	Chain	Length	Quality of chain
2	O	238	 75% 18% . . .
2	P	238	 72% 20% . . .
2	Q	238	 76% 18% . . .
2	R	238	 72% 22% . .

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	233	1838	1168	336	327	7	0	0	0
2	N	233	1838	1168	336	327	7	0	0	0
2	O	233	1838	1168	336	327	7	0	0	0
2	P	233	1838	1168	336	327	7	0	0	0
2	Q	233	1838	1168	336	327	7	0	0	0
2	R	233	1838	1168	336	327	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

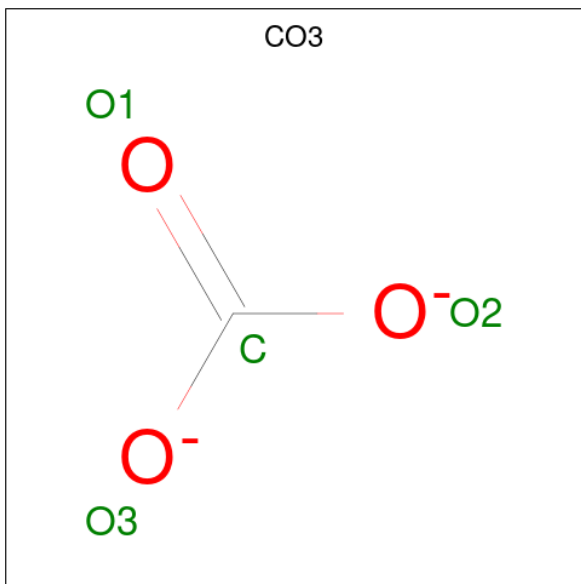
Chain	Residue	Modelled	Actual	Comment	Reference
M	447	HIS	TYR	engineered mutation	UNP P00437

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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 (three-letter code: CO3) (formula: CO₃).

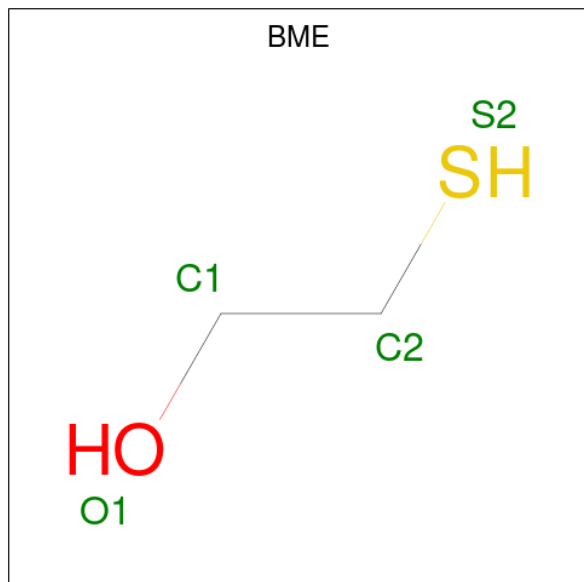


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	M	1	4	1	3	0	0
3	N	1	4	1	3	0	0
3	O	1	4	1	3	0	0
3	P	1	4	1	3	0	0
3	Q	1	4	1	3	0	0
3	R	1	4	1	3	0	0

- Molecule 4 is FE (III) ION (three-letter code: 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 (three-letter code: 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.

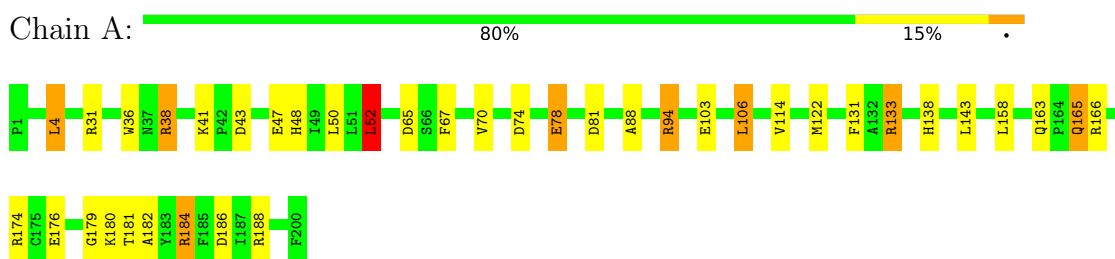
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	73	Total O 73 73	0	0
6	M	161	Total O 161 161	0	0
6	B	79	Total O 79 79	0	0
6	N	163	Total O 163 163	0	0
6	C	78	Total O 78 78	0	0
6	O	156	Total O 156 156	0	0
6	D	81	Total O 81 81	0	0
6	P	151	Total O 151 151	0	0
6	E	82	Total O 82 82	0	0
6	Q	159	Total O 159 159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

3 Residue-property plots [i](#)

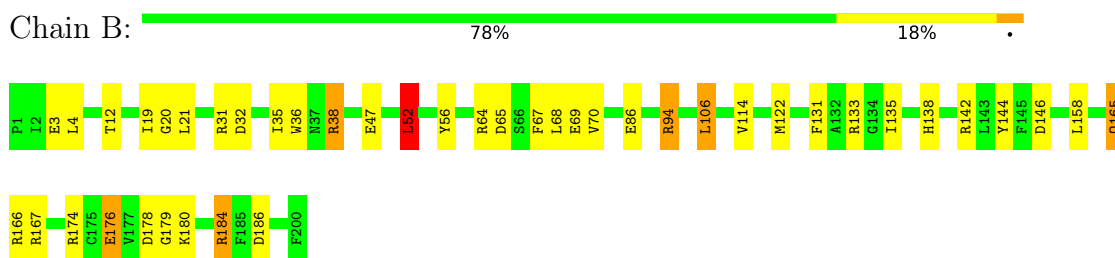
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

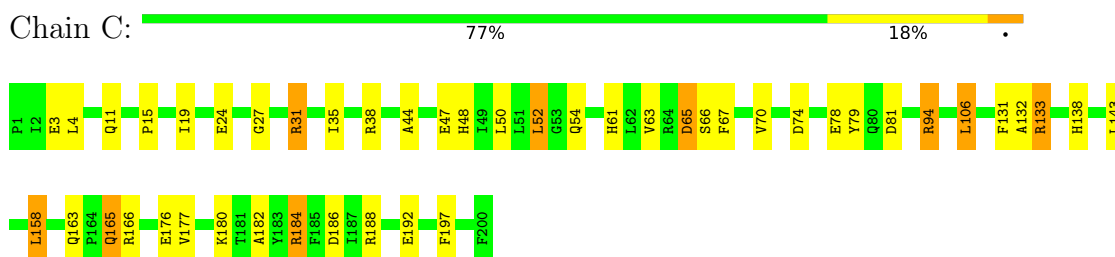
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



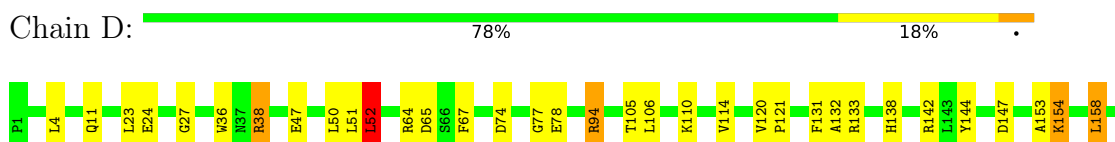
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

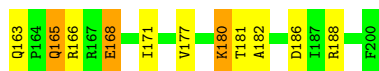


- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



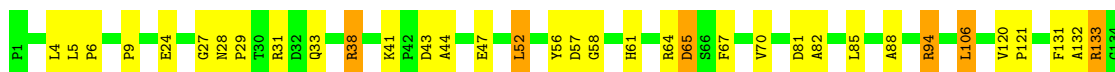
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 72% 23% 5%



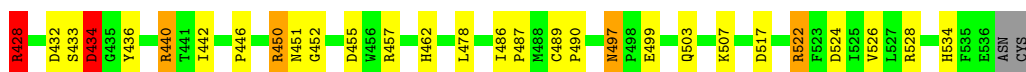
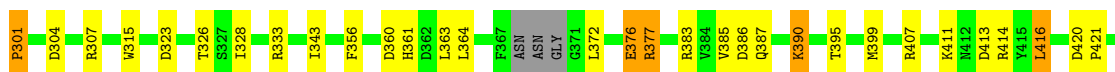
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 72% 22% 6%



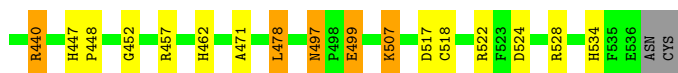
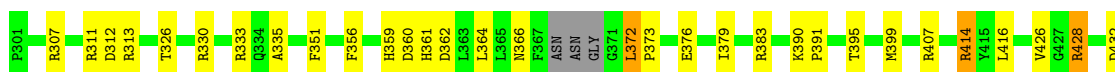
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 73% 21% ..



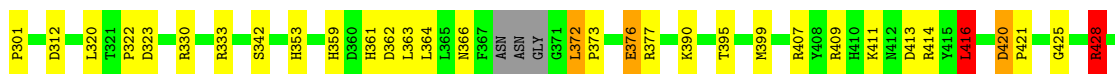
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

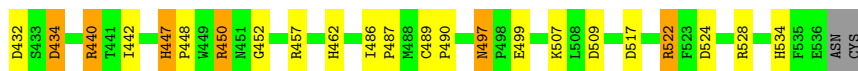
Chain N: 78% 17% ..



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

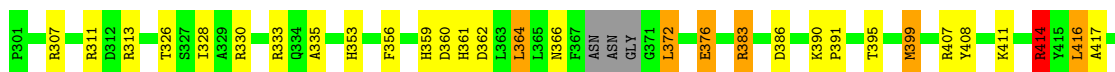
Chain O: 75% 18% ..





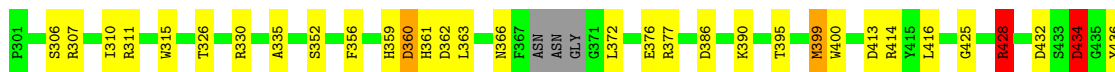
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 72% 20% . . .



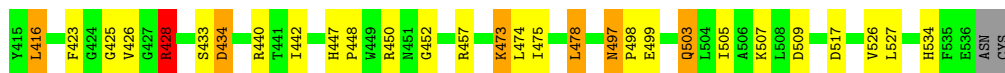
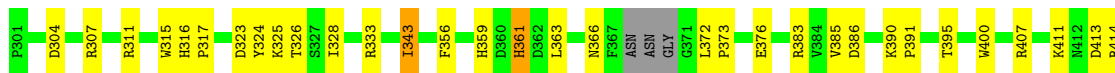
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 76% 18% . . .



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 72% 22% . .



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
Total number of atoms	21930	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.05	1/1611 (0.1%)	1.70	30/2195 (1.4%)
1	B	1.06	2/1611 (0.1%)	1.79	30/2195 (1.4%)
1	C	1.04	0/1611	1.71	26/2195 (1.2%)
1	D	1.06	2/1611 (0.1%)	1.78	28/2195 (1.3%)
1	E	1.01	1/1611 (0.1%)	1.60	28/2195 (1.3%)
1	F	1.03	0/1611	1.65	25/2195 (1.1%)
2	M	1.12	1/1893 (0.1%)	1.67	35/2577 (1.4%)
2	N	1.08	2/1893 (0.1%)	1.63	36/2577 (1.4%)
2	O	1.11	2/1893 (0.1%)	1.56	32/2577 (1.2%)
2	P	1.12	1/1893 (0.1%)	1.75	34/2577 (1.3%)
2	Q	1.14	3/1893 (0.2%)	1.70	27/2577 (1.0%)
2	R	1.14	2/1893 (0.1%)	1.62	30/2577 (1.2%)
All	All	1.08	17/21024 (0.1%)	1.68	361/28632 (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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	ARG	CD-NE	-7.01	1.34	1.46
1	A	94	ARG	CD-NE	-6.94	1.34	1.46
2	R	452	GLY	N-CA	6.50	1.55	1.46
2	Q	466	SER	CB-OG	6.26	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	440	ARG	CD-NE	-6.24	1.35	1.46
2	P	428	ARG	CD-NE	-6.19	1.35	1.46
2	N	440	ARG	CD-NE	-5.90	1.36	1.46
2	Q	428	ARG	CD-NE	-5.87	1.36	1.46
1	D	133	ARG	CD-NE	-5.75	1.36	1.46
2	N	428	ARG	CD-NE	-5.50	1.37	1.46
2	O	342	SER	CB-OG	5.33	1.49	1.42
1	B	94	ARG	CD-NE	-5.30	1.37	1.46
1	B	69	GLU	CD-OE2	-5.17	1.20	1.25
2	R	428	ARG	CD-NE	-5.13	1.37	1.46
1	E	94	ARG	CD-NE	-5.08	1.37	1.46
2	M	440	ARG	CD-NE	-5.08	1.37	1.46
2	O	440	ARG	CD-NE	-5.07	1.37	1.46

All (361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	NE-CZ-NH2	-31.69	104.46	120.30
1	D	133	ARG	CD-NE-CZ	30.52	166.32	123.60
1	B	133	ARG	CD-NE-CZ	29.97	165.56	123.60
2	N	440	ARG	NE-CZ-NH2	-22.92	108.84	120.30
2	P	440	ARG	NE-CZ-NH1	22.20	131.40	120.30
2	R	440	ARG	NE-CZ-NH2	-20.39	110.11	120.30
2	M	440	ARG	NE-CZ-NH2	-20.38	110.11	120.30
2	Q	457	ARG	NE-CZ-NH1	20.22	130.41	120.30
1	C	94	ARG	NE-CZ-NH2	-19.67	110.46	120.30
1	D	94	ARG	NE-CZ-NH2	-19.26	110.67	120.30
1	C	94	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	B	184	ARG	NE-CZ-NH2	-18.23	111.19	120.30
1	C	133	ARG	NE-CZ-NH1	17.27	128.93	120.30
1	A	94	ARG	CD-NE-CZ	17.01	147.42	123.60
1	B	94	ARG	NE-CZ-NH1	16.76	128.68	120.30
2	P	428	ARG	NE-CZ-NH1	15.67	128.14	120.30
2	Q	440	ARG	NE-CZ-NH2	-15.35	112.62	120.30
2	O	440	ARG	NE-CZ-NH2	-15.27	112.67	120.30
1	C	133	ARG	CD-NE-CZ	15.17	144.83	123.60
2	N	428	ARG	NE-CZ-NH1	15.04	127.82	120.30
1	F	166	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	D	94	ARG	NE-CZ-NH1	14.77	127.68	120.30
1	F	94	ARG	NE-CZ-NH1	14.38	127.49	120.30
1	E	133	ARG	CD-NE-CZ	14.38	143.72	123.60
2	M	450	ARG	NE-CZ-NH1	14.07	127.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	F	166	ARG	NE-CZ-NH1	13.67	127.14	120.30
2	Q	457	ARG	NE-CZ-NH2	-13.48	113.56	120.30
2	Q	428	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	A	133	ARG	CD-NE-CZ	13.41	142.38	123.60
1	F	94	ARG	NE-CZ-NH2	-13.23	113.69	120.30
1	E	94	ARG	NE-CZ-NH1	13.17	126.88	120.30
1	D	94	ARG	CD-NE-CZ	13.12	141.97	123.60
1	D	133	ARG	NE-CZ-NH1	13.06	126.83	120.30
2	P	428	ARG	NE-CZ-NH2	-12.54	114.03	120.30
2	R	407	ARG	NE-CZ-NH1	12.37	126.49	120.30
2	Q	531	ARG	NE-CZ-NH1	12.32	126.46	120.30
2	N	440	ARG	NE-CZ-NH1	12.19	126.40	120.30
2	R	457	ARG	NE-CZ-NH1	12.13	126.36	120.30
2	Q	311	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	A	94	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	B	94	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	C	188	ARG	NE-CZ-NH1	11.88	126.24	120.30
2	O	457	ARG	NE-CZ-NH1	11.82	126.21	120.30
2	N	428	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	E	133	ARG	NE-CZ-NH1	11.40	126.00	120.30
2	P	428	ARG	CG-CD-NE	11.39	135.72	111.80
1	A	38	ARG	NE-CZ-NH2	-11.38	114.61	120.30
2	R	428	ARG	CD-NE-CZ	11.32	139.46	123.60
2	M	457	ARG	NE-CZ-NH1	11.25	125.92	120.30
2	Q	311	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	D	47	GLU	CA-CB-CG	11.14	137.90	113.40
2	R	428	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	B	38	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	C	133	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	A	188	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	D	94	ARG	CG-CD-NE	10.64	134.14	111.80
1	D	38	ARG	NE-CZ-NH1	10.61	125.61	120.30
2	M	428	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	B	184	ARG	NE-CZ-NH1	10.57	125.58	120.30
2	Q	440	ARG	NE-CZ-NH1	10.57	125.58	120.30
2	Q	522	ARG	NE-CZ-NH1	-10.55	115.02	120.30
2	Q	428	ARG	CD-NE-CZ	10.53	138.34	123.60
2	M	307	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	F	188	ARG	NE-CZ-NH1	10.11	125.36	120.30
1	A	38	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	B	31	ARG	NE-CZ-NH1	9.82	125.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	ARG	NE-CZ-NH1	9.79	125.20	120.30
2	M	434	ASP	CB-CG-OD2	-9.69	109.58	118.30
2	M	450	ARG	CD-NE-CZ	9.62	137.07	123.60
2	O	428	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	P	428	ARG	CD-NE-CZ	9.52	136.93	123.60
2	P	457	ARG	NE-CZ-NH1	9.36	124.98	120.30
2	Q	428	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	E	142	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	A	184	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	C	188	ARG	NE-CZ-NH2	-9.21	115.70	120.30
1	A	94	ARG	CG-CD-NE	9.15	131.02	111.80
1	A	74	ASP	CB-CG-OD1	9.14	126.53	118.30
2	N	428	ARG	CG-CD-NE	9.12	130.96	111.80
2	Q	434	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	F	47	GLU	CA-CB-CG	8.98	133.16	113.40
1	C	184	ARG	NE-CZ-NH2	-8.96	115.82	120.30
2	N	457	ARG	NE-CZ-NH2	-8.94	115.83	120.30
2	O	524	ASP	CB-CG-OD1	8.90	126.31	118.30
2	M	524	ASP	CB-CG-OD1	8.87	126.28	118.30
1	C	94	ARG	CD-NE-CZ	8.83	135.96	123.60
2	R	311	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	D	64	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	O	428	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	M	414	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	166	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	E	38	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	M	377	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	E	94	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	E	142	ARG	NE-CZ-NH1	8.63	124.61	120.30
2	M	428	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	B	146	ASP	CB-CG-OD1	8.58	126.03	118.30
1	C	47	GLU	CA-CB-CG	8.57	132.26	113.40
2	R	440	ARG	NH1-CZ-NH2	8.52	128.77	119.40
2	P	313	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	B	106	LEU	CA-CB-CG	8.31	134.40	115.30
2	Q	311	ARG	CD-NE-CZ	8.29	135.21	123.60
2	M	333	ARG	NE-CZ-NH2	-8.25	116.18	120.30
2	N	528	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	F	106	LEU	CA-CB-CG	8.16	134.06	115.30
1	E	188	ARG	NE-CZ-NH1	8.01	124.31	120.30
2	O	330	ARG	NE-CZ-NH2	-7.99	116.31	120.30
2	M	428	ARG	CD-NE-CZ	7.91	134.68	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	CG-CD-NE	7.89	128.37	111.80
2	R	376	GLU	OE1-CD-OE2	7.85	132.72	123.30
2	N	524	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	65	ASP	CB-CG-OD1	7.75	125.28	118.30
2	O	528	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	E	94	ARG	CG-CD-NE	7.70	127.97	111.80
1	C	166	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	N	457	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	C	81	ASP	CB-CG-OD1	7.59	125.13	118.30
1	F	38	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	P	414	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	D	65	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	47	GLU	CA-CB-CG	7.52	129.94	113.40
2	R	450	ARG	CD-NE-CZ	-7.51	113.09	123.60
2	R	428	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	142	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	O	353	HIS	CA-CB-CG	-7.39	101.03	113.60
1	E	186	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	188	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	Q	377	ARG	NE-CZ-NH1	-7.37	116.61	120.30
2	R	323	ASP	CB-CG-OD1	7.36	124.93	118.30
2	O	434	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	C	65	ASP	CB-CG-OD1	7.32	124.89	118.30
2	Q	524	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	C	31	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	Q	330	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	F	74	ASP	CB-CG-OD1	7.21	124.79	118.30
2	M	376	GLU	OE1-CD-OE2	7.17	131.91	123.30
1	A	74	ASP	CB-CG-OD2	-7.16	111.85	118.30
2	M	457	ARG	CD-NE-CZ	7.13	133.59	123.60
2	O	522	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	D	38	ARG	CD-NE-CZ	7.12	133.56	123.60
2	M	432	ASP	CB-CG-OD1	7.05	124.64	118.30
2	P	483	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	94	ARG	CB-CG-CD	7.04	129.89	111.60
2	P	432	ASP	CB-CG-OD1	6.99	124.59	118.30
2	M	528	ARG	NE-CZ-NH1	-6.99	116.81	120.30
2	R	311	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	106	LEU	CA-CB-CG	6.96	131.32	115.30
2	P	528	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	R	428	ARG	CG-CD-NE	6.91	126.31	111.80
1	A	166	ARG	NE-CZ-NH1	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	440	ARG	CD-NE-CZ	6.84	133.18	123.60
2	N	414	ARG	NE-CZ-NH1	6.81	123.71	120.30
2	N	313	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	O	333	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	36	TRP	CB-CA-C	6.75	123.90	110.40
2	N	414	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	Q	307	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	O	517	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	186	ASP	CB-CG-OD1	6.71	124.33	118.30
1	C	78	GLU	OE1-CD-OE2	6.70	131.34	123.30
2	O	432	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	174	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	R	517	ASP	CB-CG-OD1	6.67	124.30	118.30
2	N	507	LYS	CA-CB-CG	6.66	128.05	113.40
1	C	186	ASP	CB-CG-OD1	6.65	124.28	118.30
1	D	94	ARG	CB-CG-CD	6.63	128.83	111.60
2	N	383	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	184	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	94	ARG	CD-NE-CZ	6.57	132.80	123.60
2	M	432	ASP	CB-CG-OD2	-6.54	112.42	118.30
2	P	524	ASP	CB-CG-OD1	6.54	124.18	118.30
2	R	383	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	R	473	LYS	CA-CB-CG	6.49	127.69	113.40
2	P	434	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	11	GLN	N-CA-CB	6.46	122.23	110.60
1	B	52	LEU	CB-CA-C	6.46	122.47	110.20
2	O	312	ASP	CB-CG-OD1	6.44	124.09	118.30
2	M	440	ARG	NH1-CZ-NH2	6.43	126.47	119.40
2	M	524	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	N	311	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	O	509	ASP	CB-CG-OD1	6.40	124.06	118.30
2	N	517	ASP	CB-CG-OD1	6.38	124.04	118.30
1	E	64	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	E	64	ARG	NE-CZ-NH1	-6.38	117.11	120.30
2	Q	531	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	F	133	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	158	LEU	CB-CA-C	6.35	122.27	110.20
1	D	186	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	E	81	ASP	CB-CG-OD1	6.34	124.01	118.30
1	F	65	ASP	CB-CG-OD1	6.34	124.01	118.30
1	C	106	LEU	CA-CB-CG	6.34	129.88	115.30
2	P	383	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CB-CG-OD2	-6.32	112.61	118.30
2	M	383	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	188	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	P	386	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	166	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	E	52	LEU	CB-CA-C	6.23	122.03	110.20
2	O	447	HIS	N-CA-CB	6.22	121.79	110.60
1	A	174	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	P	333	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	E	65	ASP	CB-CG-OD1	6.20	123.88	118.30
2	O	420	ASP	CB-CG-OD1	6.17	123.85	118.30
1	E	56	TYR	CB-CG-CD1	-6.16	117.31	121.00
1	E	94	ARG	CD-NE-CZ	6.15	132.21	123.60
1	F	52	LEU	CB-CA-C	6.13	121.85	110.20
1	B	186	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	O	323	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	197	PHE	CB-CG-CD1	-6.04	116.57	120.80
2	P	524	ASP	CB-CG-OD2	-6.01	112.89	118.30
2	P	383	ARG	NE-CZ-NH1	-6.00	117.30	120.30
2	R	450	ARG	NE-CZ-NH1	-6.00	117.30	120.30
2	O	416	LEU	CB-CA-C	5.99	121.58	110.20
1	B	178	ASP	CB-CA-C	5.98	122.36	110.40
2	O	407	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	E	31	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	R	428	ARG	CB-CG-CD	5.96	127.09	111.60
2	O	377	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	F	158	LEU	CA-CB-CG	5.92	128.92	115.30
2	R	407	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	Q	432	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	94	ARG	CB-CG-CD	5.91	126.98	111.60
1	B	166	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	E	133	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	N	432	ASP	CB-CG-OD1	5.88	123.59	118.30
2	O	440	ARG	NH1-CZ-NH2	5.88	125.87	119.40
1	B	186	ASP	CB-CG-OD1	5.86	123.58	118.30
2	Q	360	ASP	CB-CG-OD2	-5.86	113.02	118.30
2	O	517	ASP	CB-CG-OD2	-5.85	113.03	118.30
2	N	471	ALA	N-CA-CB	5.84	118.28	110.10
1	F	177	VAL	CB-CA-C	5.81	122.44	111.40
1	C	166	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	Q	524	ASP	CB-CG-OD1	5.80	123.52	118.30
2	R	383	ARG	NE-CZ-NH1	-5.80	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	103	GLU	CG-CD-OE1	-5.79	106.72	118.30
2	P	517	ASP	CB-CG-OD1	5.79	123.51	118.30
2	P	307	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	176	GLU	CB-CG-CD	5.76	129.75	114.20
2	P	353	HIS	CA-CB-CG	-5.76	103.81	113.60
1	C	74	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	184	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	O	522	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	E	184	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	R	361	HIS	CA-CB-CG	-5.72	103.87	113.60
1	F	188	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	94	ARG	CB-CG-CD	5.71	126.46	111.60
2	N	452	GLY	N-CA-C	-5.71	98.83	113.10
2	M	411	LYS	CB-CA-C	-5.67	99.05	110.40
2	M	517	ASP	CB-CG-OD1	5.67	123.40	118.30
1	F	36	TRP	CB-CA-C	5.66	121.72	110.40
2	M	407	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	F	31	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	P	408	TYR	CB-CG-CD1	-5.64	117.61	121.00
2	R	307	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	P	457	ARG	CD-NE-CZ	5.61	131.45	123.60
1	B	36	TRP	CB-CA-C	5.61	121.61	110.40
2	P	383	ARG	NH1-CZ-NH2	5.60	125.56	119.40
2	R	509	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	78	GLU	OE1-CD-OE2	5.58	129.99	123.30
2	M	450	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	64	ARG	CD-NE-CZ	-5.56	115.82	123.60
2	O	457	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	133	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	94	ARG	CB-CG-CD	5.55	126.04	111.60
2	N	372	LEU	CB-CG-CD1	5.55	120.44	111.00
2	N	407	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	57	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	P	311	ARG	CD-NE-CZ	5.54	131.36	123.60
2	O	409	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	167	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	R	376	GLU	CG-CD-OE2	-5.52	107.25	118.30
2	P	536	GLU	CG-CD-OE1	5.52	129.33	118.30
1	E	186	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	P	414	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	52	LEU	CB-CA-C	5.51	120.67	110.20
2	R	383	ARG	NH1-CZ-NH2	5.51	125.46	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	TRP	CB-CA-C	5.50	121.41	110.40
1	F	140	HIS	CB-CA-C	-5.50	99.39	110.40
2	M	413	ASP	CB-CG-OD1	5.50	123.25	118.30
2	R	304	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	N	312	ASP	CB-CG-OD1	5.49	123.24	118.30
2	N	307	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	N	428	ARG	CB-CG-CD	5.48	125.86	111.60
1	C	186	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	Q	386	ASP	CB-CA-C	5.48	121.36	110.40
2	M	452	GLY	N-CA-C	-5.48	99.41	113.10
1	D	64	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	R	324	TYR	CB-CG-CD2	5.47	124.28	121.00
2	Q	442	ILE	CA-CB-CG2	5.47	121.84	110.90
2	M	522	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	E	82	ALA	CB-CA-C	5.46	118.29	110.10
1	F	43	ASP	CB-CG-OD2	-5.45	113.39	118.30
2	M	376	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	E	183	TYR	CA-CB-CG	5.44	123.74	113.40
1	C	158	LEU	CB-CA-C	5.44	120.53	110.20
2	N	524	ASP	CB-CG-OD1	5.44	123.19	118.30
2	Q	428	ARG	CG-CD-NE	5.42	123.19	111.80
2	N	499	GLU	CG-CD-OE1	5.42	129.15	118.30
1	B	56	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	M	457	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	178	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	78	GLU	CG-CD-OE2	-5.41	107.48	118.30
1	B	38	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	74	ASP	CB-CG-OD1	5.40	123.16	118.30
2	O	452	GLY	N-CA-C	-5.39	99.63	113.10
2	R	323	ASP	CB-CG-OD2	-5.38	113.45	118.30
2	N	360	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	F	158	LEU	CB-CA-C	5.36	120.39	110.20
2	O	407	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	P	509	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	F	142	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	158	LEU	CA-CB-CG	5.35	127.60	115.30
2	N	372	LEU	CA-CB-CG	5.34	127.59	115.30
2	P	372	LEU	CB-CG-CD1	5.34	120.08	111.00
2	O	450	ARG	CD-NE-CZ	-5.34	116.12	123.60
2	O	440	ARG	CB-CG-CD	-5.34	97.72	111.60
2	P	383	ARG	CD-NE-CZ	-5.32	116.16	123.60
2	M	390	LYS	CA-CB-CG	5.32	125.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	LEU	CB-CA-C	5.30	120.28	110.20
2	M	323	ASP	CB-CG-OD1	5.28	123.05	118.30
2	N	440	ARG	CB-CG-CD	-5.28	97.88	111.60
1	B	65	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	31	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	Q	432	ASP	CB-CG-OD2	-5.26	113.56	118.30
2	N	333	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	R	434	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	F	103	GLU	CG-CD-OE2	5.22	128.75	118.30
2	N	522	ARG	CD-NE-CZ	5.21	130.90	123.60
1	B	86	GLU	CG-CD-OE1	5.21	128.71	118.30
2	P	376	GLU	CG-CD-OE2	-5.20	107.91	118.30
1	E	106	LEU	CA-CB-CG	5.18	127.21	115.30
2	N	311	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	N	312	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	133	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	103	GLU	CG-CD-OE1	-5.15	108.00	118.30
1	E	52	LEU	CA-CB-CG	5.14	127.13	115.30
2	M	383	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	M	383	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	F	38	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	N	311	ARG	CD-NE-CZ	5.13	130.78	123.60
1	D	168	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	E	174	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	132	ALA	N-CA-CB	5.12	117.26	110.10
2	N	376	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	C	94	ARG	CG-CD-NE	5.10	122.50	111.80
1	D	23	LEU	CB-CA-C	5.10	119.88	110.20
2	O	447	HIS	O-C-N	5.09	130.78	121.10
2	M	377	ARG	CD-NE-CZ	-5.09	116.48	123.60
1	F	141	THR	CA-CB-CG2	5.08	119.52	112.40
1	B	176	GLU	CG-CD-OE1	5.08	128.46	118.30
2	O	376	GLU	OE1-CD-OE2	5.08	129.40	123.30
2	P	509	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	11	GLN	O-C-N	5.07	130.81	122.70
2	R	411	LYS	CB-CA-C	-5.06	100.28	110.40
2	N	383	ARG	N-CA-CB	-5.06	101.50	110.60
1	D	142	ARG	CA-CB-CG	5.05	124.51	113.40
1	A	186	ASP	CB-CG-OD1	5.01	122.81	118.30
2	P	311	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	174	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	Q	307	ARG	NE-CZ-NH2	-5.01	117.80	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	P	440	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	28	0
1	B	1571	0	1499	26	0
1	C	1571	0	1499	33	0
1	D	1571	0	1499	23	0
1	E	1571	0	1499	42	0
1	F	1571	0	1499	44	0
2	M	1838	0	1791	44	0
2	N	1838	0	1791	21	0
2	O	1838	0	1791	31	0
2	P	1838	0	1791	42	0
2	Q	1838	0	1791	35	0
2	R	1838	0	1791	37	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
6	O	156	0	0	2	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	377	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 9.

All (377) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:176:GLU:HG3	1:B:180:LYS:C	2.08	0.74
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
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:O:413:ASP:C	2:O:414:ARG:HD2	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.63	0.64
2:P:361:HIS:H	2:P:361:HIS:HD2	1.44	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
2:O:416:LEU:C	2:O:416:LEU:HD23	2.20	0.61
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: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
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: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
2:R:413:ASP:C	2:R:414:ARG:HD2	2.23	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:P:478:LEU:C	2:P:478:LEU:HD23	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:A:114:VAL:HG23	1:A:122:MET:CE	2.37	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: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
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.27	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
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.90	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
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.24	0.53
1:B:144:TYR:CE1	1:B:158:LEU:HD13	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.72	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
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
2:P:416:LEU:C	2:P:416:LEU:HD23	2.30	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
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:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.11	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:413:ASP:O	2:O:414:ARG:HD2	2.11	0.50
1:D:51:LEU:O	1:D:105:THR:HA	2.11	0.50
1:C:143:LEU:HD23	1:C:143:LEU:C	2.32	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:A:114:VAL:HG23	1:A:122:MET:HE3	1.93	0.49
2:M:416:LEU:C	2:M:416:LEU:CD2	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.15	0.49
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.42	0.49
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.95	0.49
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.33	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:A:50:LEU:O	1:A:182:ALA:HA	2.13	0.49
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: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
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:F:176:GLU:OE2	1:F:179:GLY:C	2.52	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
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.77	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:R:497:ASN:HD22	2:R:497:ASN:C	2.18	0.47
2:P:411:LYS:O	2:P:414:ARG:NH1	2.44	0.47
1:E:176:GLU:HA	1:E:180:LYS:O	2.15	0.47
2:R:416:LEU:C	2:R:416:LEU:HD23	2.34	0.47
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.96	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
2:R:478:LEU:C	2:R:478:LEU:HD23	2.35	0.47
1:C:24:GLU:O	1:C:27:GLY:N	2.44	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
2:N:478:LEU:C	2:N:478:LEU:HD23	2.35	0.46
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.30	0.46
1:A:143:LEU:C	1:A:143:LEU:HD23	2.35	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
2:M:478:LEU:HD23	2:M:478:LEU:C	2.35	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:R:400:TRP:HA	2:R:425:GLY:O	2.16	0.46
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:B:19:ILE:O	2:N:426:VAL:HG21	2.17	0.45
2:O:416:LEU:C	2:O:416:LEU:CD2	2.84	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:E:58:GLY:CA	1:E:190:GLN:HB3	2.46	0.45
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.98	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:176:GLU:OE2	1:B:179:GLY:C	2.55	0.44
1:E:176:GLU:HG2	1:E:179:GLY:C	2.38	0.44
1:B:12:THR:HA	1:B:135:ILE:O	2.17	0.44
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
1:B:176:GLU:HG2	1:B:179:GLY:HA2	2.00	0.44
1:F:52:LEU:C	1:F:52:LEU:HD22	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LEU:C	1:F:143:LEU:HD23	2.37	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:E:174:ARG:HH21	1:E:181:THR:HG21	1.82	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
2:P:447:HIS:NE2	3:P:550:CO3:O2	2.42	0.44
2:R:473:LYS:NZ	6:R:1368:HOH:O	2.36	0.44
1:B:52:LEU:C	1:B:52:LEU:HD22	2.38	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
1:C:79:TYR:O	2:O:301:PRO:HB2	2.18	0.43
2:P:497:ASN:C	2:P:497:ASN:HD22	2.21	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: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:C:52:LEU:C	1:C:52:LEU:HD22	2.38	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:F:81:ASP:N	1:F:81:ASP:OD1	2.49	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: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
1:D:110:LYS:NZ	1:D:147:ASP:OD1	2.36	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
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:P:416:LEU:C	2:P:416:LEU:CD2	2.87	0.43
1:B:114:VAL:HG23	1:B:122:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:407:ARG:HD3	2:P:417:ALA:O	2.18	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: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: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: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
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:385:VAL:O	2:M:526:VAL:HA	2.19	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:B:35:ILE:HD13	2:N:351:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:114:VAL:CG2	1:B:122:MET:HE3	2.51	0.41
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.99	0.41
1:D:52:LEU:C	1:D:52:LEU:HD22	2.42	0.41
2:P:437:TYR:CD1	2:P:437:TYR:C	2.94	0.41
2:P:497:ASN:O	2:P:500:ALA:HB3	2.21	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
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
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.84	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 [i](#)

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%)	156 (96%)	6 (4%)	34	35
1	B	162/163 (99%)	157 (97%)	5 (3%)	40	43
1	C	162/163 (99%)	156 (96%)	6 (4%)	34	35
1	D	162/163 (99%)	155 (96%)	7 (4%)	29	29
1	E	162/163 (99%)	154 (95%)	8 (5%)	25	23
1	F	162/163 (99%)	155 (96%)	7 (4%)	29	29
2	M	196/202 (97%)	185 (94%)	11 (6%)	21	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	196/202 (97%)	187 (95%)	9 (5%)	27	26
2	O	196/202 (97%)	188 (96%)	8 (4%)	30	31
2	P	196/202 (97%)	183 (93%)	13 (7%)	16	14
2	Q	196/202 (97%)	185 (94%)	11 (6%)	21	18
2	R	196/202 (97%)	184 (94%)	12 (6%)	18	16
All	All	2148/2190 (98%)	2045 (95%)	103 (5%)	25	24

All (103) 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	165	GLN
2	M	301	PRO
2	M	372	LEU
2	M	386	ASP
2	M	395	THR
2	M	416	LEU
2	M	428	ARG
2	M	433	SER
2	M	434	ASP
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	373	PRO
2	N	395	THR
2	N	416	LEU
2	N	478	LEU
2	N	497	ASN
2	N	507	LYS

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Mol	Chain	Res	Type
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	165	GLN
1	C	192	GLU
2	O	372	LEU
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	38	ARG
1	D	52	LEU
1	D	106	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	372	LEU
2	P	395	THR
2	P	399	MET
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	497	ASN
2	P	503	GLN
2	P	534	HIS
1	E	4	LEU
1	E	9	PRO
1	E	38	ARG
1	E	43	ASP
1	E	47	GLU
1	E	52	LEU
1	E	165	GLN

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Mol	Chain	Res	Type
1	E	180	LYS
2	Q	352	SER
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	478	LEU
2	Q	497	ASN
2	Q	503	GLN
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	38	ARG
1	F	52	LEU
1	F	165	GLN
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	428	ARG
2	R	433	SER
2	R	434	ASP
2	R	442	ILE
2	R	478	LEU
2	R	497	ASN
2	R	503	GLN
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	165	GLN

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Mol	Chain	Res	Type
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	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 monosaccharides 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	O	550	4	2,3,3	0.61	0	2,3,3	1.43	0
5	BME	Q	601	2	3,3,3	0.57	0	1,2,2	1.15	0
3	CO3	R	550	4	2,3,3	0.63	0	2,3,3	1.77	1 (50%)
3	CO3	M	550	4	2,3,3	0.39	0	2,3,3	1.05	0
5	BME	P	601	2	3,3,3	0.44	0	1,2,2	1.15	0
5	BME	N	601	2	3,3,3	0.25	0	1,2,2	0.51	0
3	CO3	P	550	4	2,3,3	0.46	0	2,3,3	0.69	0
5	BME	O	601	2	3,3,3	0.35	0	1,2,2	1.00	0
3	CO3	N	550	4	2,3,3	0.32	0	2,3,3	1.11	0
5	BME	R	601	2	3,3,3	0.30	0	1,2,2	0.07	0
3	CO3	Q	550	4	2,3,3	0.78	0	2,3,3	3.22	2 (100%)
5	BME	M	601	2	3,3,3	0.38	0	1,2,2	0.47	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BME	Q	601	2	-	0/1/1/1	-
5	BME	P	601	2	-	0/1/1/1	-
5	BME	N	601	2	-	0/1/1/1	-
5	BME	O	601	2	-	0/1/1/1	-
5	BME	R	601	2	-	0/1/1/1	-
5	BME	M	601	2	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	550	CO3	O3-C-O1	-3.66	110.06	119.55
3	Q	550	CO3	O2-C-O1	-2.70	112.54	119.55
3	R	550	CO3	O3-C-O1	-2.43	113.25	119.55

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
5	Q	601	BME	2	0
3	R	550	CO3	1	0
3	M	550	CO3	1	0
3	P	550	CO3	1	0
5	O	601	BME	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.