



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:51 PM UTC

PDB ID : 3PCB / pdb\_00003pcb  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 3-HYDROXYBENZOATE  
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.  
Deposited on : 1997-04-25  
Resolution : 2.19 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](mailto: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>.

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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)  
Xtrriage (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

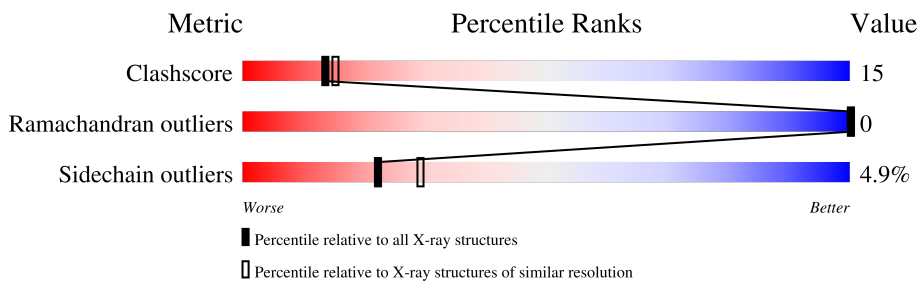
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)





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  $\geq 3$ , 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	70% 24% 6%
1	B	200	67% 24% 8%
1	C	200	68% 25% 6%
1	D	200	70% 24% 6%
1	E	200	64% 30% 6% .
1	F	200	61% 29% 9% .
2	M	238	64% 27% 6% .
2	N	238	69% 26% . .

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Mol	Chain	Length	Quality of chain
2	O	238	 65% 27% 5% •
2	P	238	 68% 23% 6% ••
2	Q	238	 66% 26% 5% •
2	R	238	 64% 27% 7% •

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22032 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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

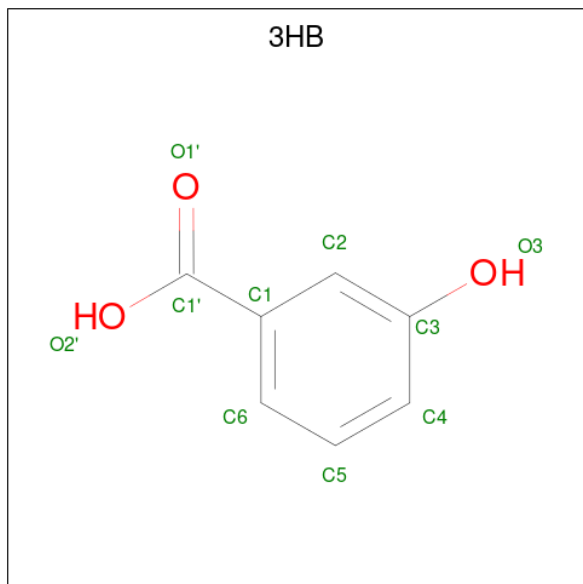
- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

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

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

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

- Molecule 4 is 3-HYDROXYBENZOIC ACID (CCD ID: 3HB) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O 10 7 3	0	0
4	M	1	Total C O 10 7 3	0	0
4	N	1	Total C O 10 7 3	0	0
4	N	1	Total C O 10 7 3	0	0
4	O	1	Total C O 10 7 3	0	0
4	O	1	Total C O 10 7 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	C	O	0	0
			10	7	3		
4	P	1	Total	C	O	0	0
			10	7	3		
4	Q	1	Total	C	O	0	0
			10	7	3		
4	Q	1	Total	C	O	0	0
			10	7	3		
4	R	1	Total	C	O	0	0
			10	7	3		
4	R	1	Total	C	O	0	0
			10	7	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	M	151	Total	O	0	0
			151	151		
5	B	79	Total	O	0	0
			79	79		
5	N	161	Total	O	0	0
			161	161		
5	C	81	Total	O	0	0
			81	81		
5	O	155	Total	O	0	0
			155	155		
5	D	81	Total	O	0	0
			81	81		
5	P	152	Total	O	0	0
			152	152		
5	E	84	Total	O	0	0
			84	84		
5	Q	153	Total	O	0	0
			153	153		
5	F	80	Total	O	0	0
			80	80		
5	R	156	Total	O	0	0
			156	156		

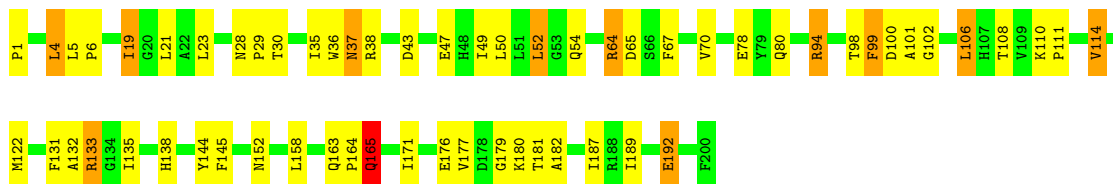
### 3 Residue-property plots [i](#)

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.

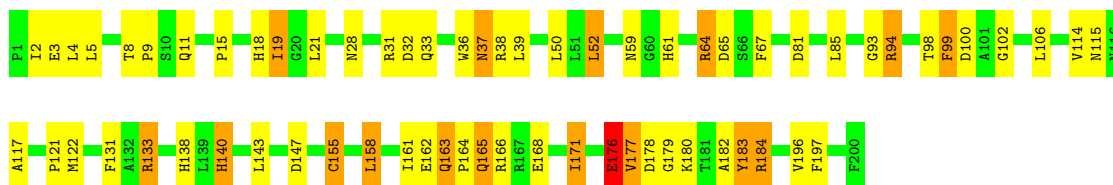
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A: 



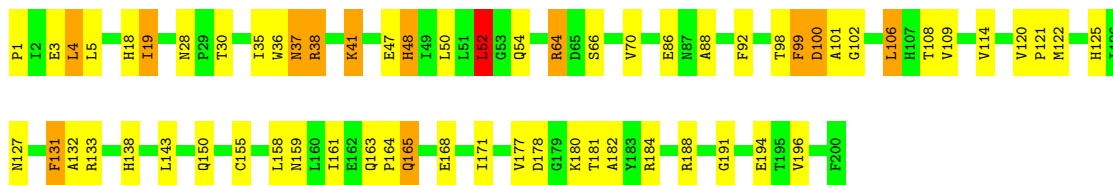
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain B: 



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

Chain C: 



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

Chain D: 

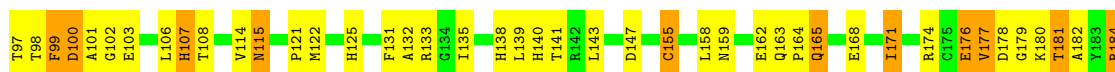




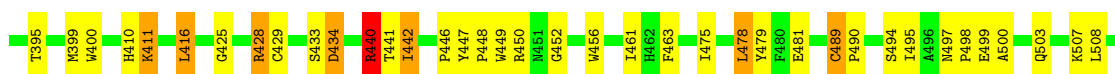
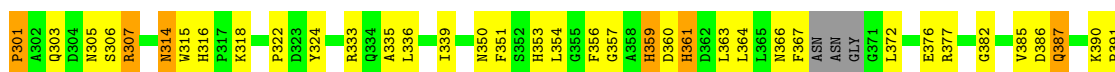
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



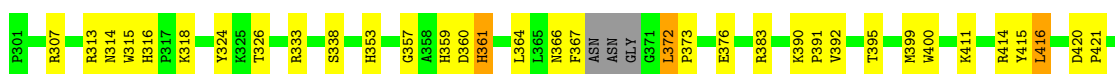
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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

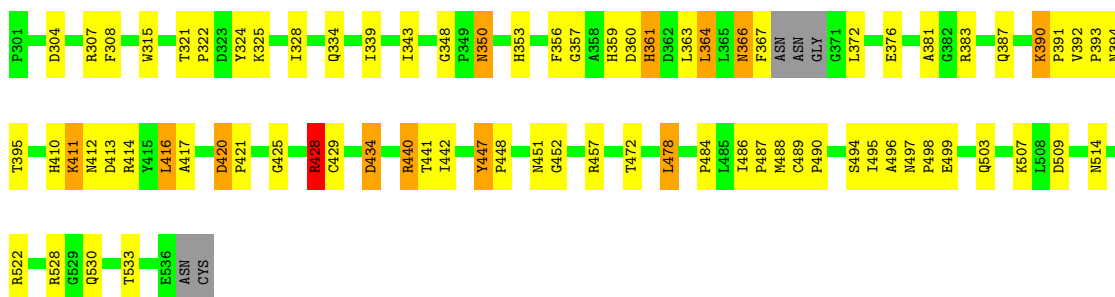


- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



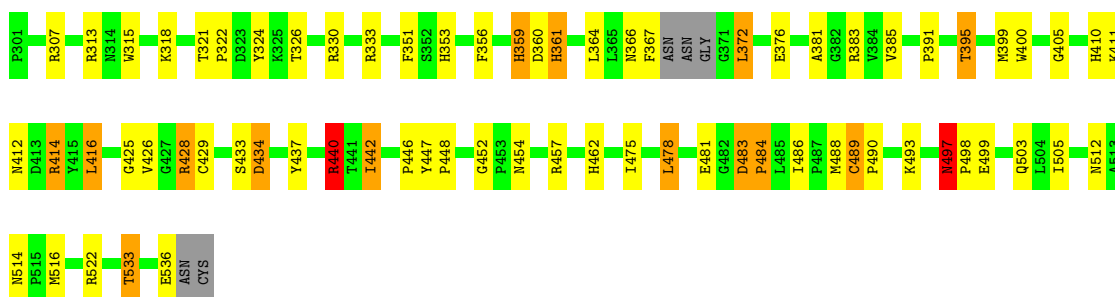
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain O:  65% 27% 5% .



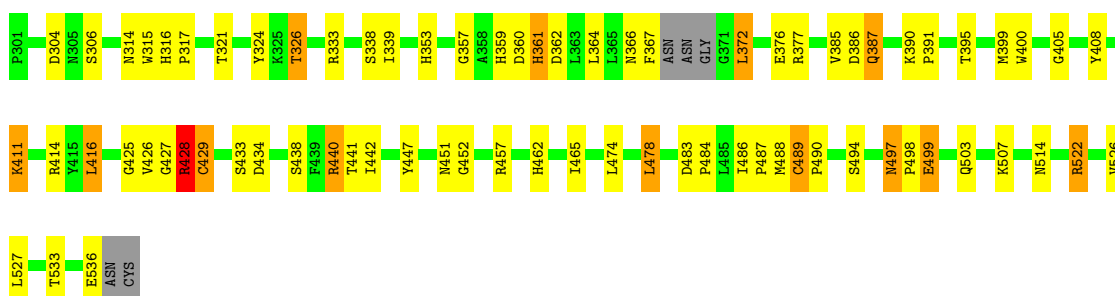
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain P:  68% 23% 6% ..



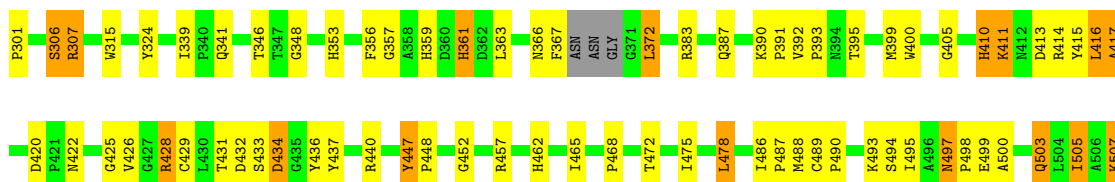
- Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain Q:  66% 26% 5% .



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

Chain R:  64% 27% 7% .





## 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, $\alpha$ , $\beta$ , $\gamma$	196.95Å 127.56Å 134.31Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.19	Depositor
% Data completeness (in resolution range)	78.2 (6.00-2.19)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: CME, FE, 3HB

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	1.20	3/1611 (0.2%)	1.81	26/2195 (1.2%)
1	B	1.18	2/1611 (0.1%)	1.82	30/2195 (1.4%)
1	C	1.26	1/1611 (0.1%)	1.80	27/2195 (1.2%)
1	D	1.24	3/1611 (0.2%)	1.86	24/2195 (1.1%)
1	E	1.28	2/1611 (0.1%)	1.82	28/2195 (1.3%)
1	F	1.33	4/1611 (0.2%)	1.82	35/2195 (1.6%)
2	M	1.29	3/1888 (0.2%)	1.82	34/2569 (1.3%)
2	N	1.27	4/1888 (0.2%)	1.82	38/2569 (1.5%)
2	O	1.28	3/1888 (0.2%)	1.86	35/2569 (1.4%)
2	P	1.26	2/1888 (0.1%)	1.82	36/2569 (1.4%)
2	Q	1.34	3/1888 (0.2%)	1.84	34/2569 (1.3%)
2	R	1.31	0/1888	1.83	31/2569 (1.2%)
All	All	1.27	30/20994 (0.1%)	1.83	378/28584 (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	F	0	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	451	ASN	CA-C	9.15	1.56	1.52
2	O	451	ASN	CA-C	8.45	1.56	1.52
1	A	94	ARG	CD-NE	-7.86	1.35	1.46
1	D	94	ARG	CD-NE	-7.72	1.35	1.46
2	Q	441	THR	CA-CB	7.06	1.63	1.53
2	P	486	ILE	CA-CB	6.82	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	441	THR	CA-CB	6.63	1.62	1.54
1	F	108	THR	CA-CB	6.59	1.63	1.54
1	B	94	ARG	CD-NE	-6.01	1.37	1.46
2	O	321	THR	N-CA	5.85	1.53	1.46
1	F	171	ILE	CA-CB	5.82	1.60	1.54
2	M	428	ARG	CD-NE	-5.72	1.38	1.46
1	D	133	ARG	CD-NE	-5.66	1.38	1.46
1	F	5	LEU	CA-C	5.56	1.58	1.53
2	N	451	ASN	CA-C	5.55	1.55	1.52
2	N	441	THR	CA-CB	5.46	1.61	1.54
1	D	189	ILE	CA-CB	5.45	1.61	1.54
1	F	135	ILE	CA-CB	5.44	1.60	1.53
2	O	441	THR	CA-CB	5.43	1.60	1.54
1	C	108	THR	CA-CB	5.32	1.61	1.54
1	B	2	ILE	CA-CB	5.31	1.60	1.54
1	A	133	ARG	CD-NE	-5.30	1.38	1.46
2	N	428	ARG	CD-NE	-5.29	1.38	1.46
2	M	359	HIS	N-CA	5.25	1.52	1.46
2	P	428	ARG	CD-NE	-5.15	1.39	1.46
2	Q	321	THR	CA-CB	5.09	1.59	1.53
2	N	440	ARG	N-CA	5.08	1.52	1.46
1	E	196	VAL	CA-C	5.05	1.58	1.52
1	E	108	THR	CA-CB	5.05	1.61	1.54
1	A	108	THR	CA-CB	5.01	1.61	1.54

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ARG	CD-NE-CZ	20.63	153.28	124.40
2	O	353	HIS	CA-CB-CG	-13.93	99.87	113.80
2	M	440	ARG	NE-CZ-NH2	-11.93	108.46	119.20
1	E	99	PHE	CA-CB-CG	11.77	125.57	113.80
2	N	440	ARG	NE-CZ-NH2	-11.49	108.86	119.20
2	R	361	HIS	CA-CB-CG	-11.43	102.37	113.80
1	A	94	ARG	CD-NE-CZ	11.40	140.37	124.40
1	D	94	ARG	NE-CZ-NH2	-10.97	109.33	119.20
2	Q	451	ASN	O-C-N	10.69	128.74	120.83
1	F	133	ARG	CD-NE-CZ	10.56	139.19	124.40
2	O	452	GLY	N-CA-C	-10.13	99.97	112.23
2	P	353	HIS	CA-CB-CG	-10.06	103.74	113.80
1	D	37	ASN	N-CA-C	9.69	123.78	112.93
1	C	99	PHE	CA-CB-CG	9.65	123.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	361	HIS	CA-CB-CG	-9.63	104.17	113.80
2	R	440	ARG	NE-CZ-NH2	-9.54	110.61	119.20
2	P	440	ARG	NE-CZ-NH2	-9.49	110.66	119.20
2	Q	452	GLY	N-CA-C	-9.47	100.77	112.23
1	A	99	PHE	CA-CB-CG	9.32	123.12	113.80
2	M	452	GLY	N-CA-C	-9.31	100.96	112.23
2	R	434	ASP	CA-CB-CG	-9.14	103.46	112.60
2	O	361	HIS	CA-CB-CG	-9.08	104.72	113.80
1	B	94	ARG	CG-CD-NE	9.01	131.81	112.00
2	R	353	HIS	CA-CB-CG	-8.99	104.81	113.80
2	R	475	ILE	N-CA-CB	8.90	123.70	111.41
2	M	353	HIS	CA-CB-CG	-8.77	105.03	113.80
1	D	99	PHE	CA-CB-CG	8.76	122.56	113.80
1	A	94	ARG	CG-CD-NE	8.61	130.95	112.00
1	F	99	PHE	CA-CB-CG	8.60	122.40	113.80
1	C	47	GLU	CB-CG-CD	8.55	127.14	112.60
2	O	428	ARG	CD-NE-CZ	8.46	136.24	124.40
2	Q	304	ASP	CA-CB-CG	8.46	121.06	112.60
1	B	94	ARG	CB-CG-CD	8.45	130.74	111.30
2	Q	361	HIS	CA-CB-CG	-8.35	105.45	113.80
2	N	452	GLY	N-CA-C	-8.34	101.84	112.10
2	O	447	TYR	O-C-N	8.28	127.64	121.85
2	N	522	ARG	CD-NE-CZ	8.24	135.94	124.40
2	Q	440	ARG	NE-CZ-NH2	-8.14	111.88	119.20
1	D	94	ARG	CG-CD-NE	8.10	129.82	112.00
1	C	37	ASN	N-CA-C	7.99	122.66	113.15
2	P	428	ARG	CG-CD-NE	7.99	129.58	112.00
1	B	99	PHE	CA-CB-CG	7.99	121.79	113.80
2	P	434	ASP	CA-CB-CG	-7.93	104.67	112.60
1	B	37	ASN	N-CA-C	7.77	122.34	113.02
1	E	64	ARG	CD-NE-CZ	-7.76	113.54	124.40
2	N	361	HIS	CA-CB-CG	-7.70	106.11	113.80
1	E	37	ASN	N-CA-C	7.64	121.49	112.93
2	M	536	GLU	CA-C-O	7.60	133.72	120.80
1	A	94	ARG	CB-CG-CD	7.58	128.72	111.30
2	N	353	HIS	CA-CB-CG	-7.54	106.26	113.80
1	B	176	GLU	CB-CG-CD	7.54	125.41	112.60
1	F	43	ASP	CA-CB-CG	-7.52	105.08	112.60
2	O	339	ILE	O-C-N	7.51	126.42	121.69
2	M	494	SER	N-CA-C	-7.50	103.39	112.54
2	R	339	ILE	O-C-N	7.49	126.41	121.69
1	F	37	ASN	N-CA-C	7.42	121.93	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	LEU	N-CA-C	-7.42	99.84	110.08
1	A	37	ASN	N-CA-C	7.42	121.24	112.93
2	M	361	HIS	CA-CB-CG	-7.41	106.39	113.80
2	M	450	ARG	CD-NE-CZ	7.38	134.72	124.40
1	A	133	ARG	CD-NE-CZ	7.37	134.72	124.40
2	O	440	ARG	NE-CZ-NH2	-7.35	112.59	119.20
1	A	5	LEU	N-CA-C	-7.35	100.50	109.83
1	D	94	ARG	NE-CZ-NH1	7.35	128.85	121.50
1	C	133	ARG	NE-CZ-NH1	7.30	128.81	121.50
1	A	94	ARG	NE-CZ-NH2	-7.28	112.64	119.20
2	P	481	GLU	CB-CG-CD	7.23	124.89	112.60
2	M	428	ARG	CB-CG-CD	7.22	127.91	111.30
2	M	441	THR	N-CA-CB	-7.15	100.36	110.51
2	Q	434	ASP	CA-CB-CG	-7.12	105.48	112.60
2	N	434	ASP	CA-CB-CG	-7.10	105.50	112.60
2	O	451	ASN	O-C-N	7.07	127.07	120.71
1	D	64	ARG	CD-NE-CZ	-6.99	114.61	124.40
2	R	457	ARG	CA-CB-CG	6.99	128.08	114.10
2	O	494	SER	N-CA-C	-6.99	103.85	112.38
1	F	94	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	C	125	HIS	CA-CB-CG	-6.95	106.85	113.80
1	B	59	ASN	OD1-CG-ND2	6.94	129.54	122.60
1	A	64	ARG	CD-NE-CZ	-6.94	114.69	124.40
1	D	28	ASN	O-C-N	6.93	127.24	121.35
1	E	5	LEU	N-CA-C	-6.93	100.52	110.08
2	M	428	ARG	CD-NE-CZ	6.87	134.02	124.40
2	R	447	TYR	O-C-N	6.84	126.64	121.85
2	P	372	LEU	CB-CA-C	6.80	118.13	108.68
2	R	422	ASN	CA-CB-CG	-6.79	105.81	112.60
2	O	434	ASP	CA-CB-CG	-6.78	105.82	112.60
2	R	348	GLY	O-C-N	6.76	128.53	121.77
1	D	133	ARG	NE-CZ-NH1	6.75	128.25	121.50
2	M	481	GLU	CB-CG-CD	6.72	124.03	112.60
1	D	94	ARG	CD-NE-CZ	6.72	133.80	124.40
2	Q	457	ARG	CD-NE-CZ	6.70	133.78	124.40
2	R	393	PRO	CA-C-N	6.68	131.84	122.36
2	R	393	PRO	C-N-CA	6.68	131.84	122.36
2	N	440	ARG	NH1-CZ-NH2	6.68	127.98	119.30
1	D	178	ASP	CA-CB-CG	-6.68	105.92	112.60
2	O	420	ASP	CB-CA-C	6.66	117.56	110.17
1	B	94	ARG	NE-CZ-NH1	6.66	128.16	121.50
2	R	494	SER	N-CA-C	-6.64	104.44	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ILE	N-CA-C	6.63	118.08	107.73
1	A	99	PHE	N-CA-C	-6.62	104.47	112.54
2	M	440	ARG	NE-CZ-NH1	6.61	128.11	121.50
2	Q	314	ASN	CB-CA-C	6.57	121.25	109.29
2	N	392	VAL	O-C-N	6.57	127.27	120.96
2	Q	339	ILE	O-C-N	6.55	125.82	121.69
2	N	514	ASN	CB-CA-C	6.54	116.65	110.17
2	N	497	ASN	CB-CA-C	6.54	118.80	109.38
1	B	64	ARG	CD-NE-CZ	-6.52	115.27	124.40
1	A	94	ARG	NE-CZ-NH1	6.52	128.02	121.50
2	R	357	GLY	N-CA-C	-6.48	104.25	112.54
2	Q	522	ARG	NE-CZ-NH1	-6.47	115.03	121.50
1	B	133	ARG	CD-NE-CZ	6.45	133.44	124.40
1	E	171	ILE	N-CA-CB	-6.42	103.70	111.21
1	C	99	PHE	N-CA-C	-6.42	104.55	112.38
2	N	514	ASN	CA-CB-CG	6.42	119.02	112.60
2	P	512	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	D	43	ASP	CA-CB-CG	-6.39	106.21	112.60
2	N	447	TYR	O-C-N	6.38	126.32	121.85
2	M	386	ASP	CA-CB-CG	6.38	118.98	112.60
2	N	357	GLY	N-CA-C	-6.37	104.03	112.82
1	C	41	LYS	N-CA-C	-6.36	100.95	110.24
2	P	489	CYS	N-CA-C	6.34	118.81	109.42
2	O	428	ARG	NE-CZ-NH1	6.34	127.84	121.50
2	Q	514	ASN	CA-CB-CG	6.32	118.92	112.60
2	M	489	CYS	O-C-N	6.31	126.67	121.31
1	B	177	VAL	CB-CA-C	6.29	118.21	110.73
2	M	428	ARG	CG-CD-NE	6.28	125.82	112.00
1	C	38	ARG	CD-NE-CZ	-6.27	115.62	124.40
2	P	536	GLU	CA-C-O	6.25	131.42	120.80
2	O	366	ASN	N-CA-C	6.24	120.75	113.20
2	R	417	ALA	N-CA-C	-6.22	101.92	109.83
2	M	307	ARG	CA-C-O	-6.21	113.84	121.11
1	C	158	LEU	N-CA-CB	-6.21	100.66	110.22
2	N	416	LEU	CB-CA-C	6.20	123.26	110.31
1	E	133	ARG	N-CA-C	-6.19	101.25	110.23
1	A	23	LEU	CB-CA-C	6.18	120.70	110.81
1	F	5	LEU	N-CA-C	-6.15	101.83	109.64
2	P	440	ARG	NE-CZ-NH1	6.12	127.62	121.50
2	O	322	PRO	CB-CA-C	6.12	121.66	111.56
1	C	133	ARG	CD-NE-CZ	6.11	132.96	124.40
2	M	411	LYS	CB-CA-C	-6.11	100.60	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	ASN	CA-CB-CG	6.11	118.71	112.60
1	F	38	ARG	CA-CB-CG	6.09	126.28	114.10
2	O	514	ASN	O-C-N	6.08	126.91	121.19
2	Q	387	GLN	OE1-CD-NE2	6.08	128.68	122.60
2	R	452	GLY	N-CA-C	-6.03	100.04	112.34
1	E	88	ALA	N-CA-C	-6.01	104.66	112.23
1	D	94	ARG	CB-CG-CD	6.01	125.12	111.30
2	P	452	GLY	N-CA-C	-6.01	100.09	112.34
1	F	107	HIS	CA-CB-CG	-6.01	107.79	113.80
1	A	192	GLU	CB-CA-C	-5.99	101.74	110.06
2	P	457	ARG	CD-NE-CZ	5.99	132.78	124.40
2	P	512	ASN	CA-CB-CG	-5.97	106.63	112.60
1	E	61	HIS	CA-CB-CG	-5.96	107.84	113.80
2	N	333	ARG	N-CA-C	-5.94	106.37	113.97
2	Q	367	PHE	CA-C-O	-5.93	110.71	120.80
1	F	90	ASN	CA-CB-CG	5.93	118.53	112.60
1	F	141	THR	CA-CB-CG2	5.93	120.58	110.50
2	Q	494	SER	N-CA-C	-5.92	105.16	112.38
2	R	387	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	B	117	ALA	CA-C-O	-5.91	114.29	120.55
2	N	440	ARG	CB-CG-CD	-5.88	97.77	111.30
1	B	133	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	47	GLU	CB-CG-CD	5.84	122.53	112.60
2	P	428	ARG	CB-CG-CD	5.84	124.73	111.30
1	E	157	VAL	CB-CA-C	5.84	119.69	112.04
2	O	348	GLY	O-C-N	5.83	127.60	121.77
2	N	523	PHE	CA-CB-CG	5.82	119.62	113.80
2	O	357	GLY	N-CA-C	-5.82	105.09	112.54
2	R	420	ASP	CB-CA-C	5.82	116.84	110.15
2	Q	353	HIS	CA-CB-CG	-5.81	107.99	113.80
1	F	125	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	133	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	F	5	LEU	O-C-N	5.80	127.28	121.30
1	C	106	LEU	N-CA-CB	-5.80	100.63	111.13
1	B	177	VAL	O-C-N	5.78	128.64	123.03
1	D	5	LEU	N-CA-C	-5.78	102.49	109.83
2	N	428	ARG	CG-CD-NE	5.77	124.70	112.00
2	P	475	ILE	N-CA-CB	5.77	119.38	111.41
1	A	30	THR	CA-CB-OG1	-5.77	100.94	109.60
2	M	333	ARG	CB-CA-C	5.77	119.79	109.29
2	O	394	ASN	CA-CB-CG	-5.77	106.83	112.60
1	E	165	GLN	OE1-CD-NE2	-5.75	116.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	NE-CZ-NH2	-5.75	114.03	119.20
1	D	23	LEU	CB-CA-C	5.74	120.05	110.92
1	B	94	ARG	CD-NE-CZ	5.74	132.44	124.40
2	O	383	ARG	NH1-CZ-NH2	5.74	126.76	119.30
2	Q	326	THR	CA-CB-OG1	-5.73	101.00	109.60
2	Q	474	LEU	N-CA-CB	-5.72	100.89	111.52
1	C	30	THR	CA-CB-OG1	-5.71	101.03	109.60
2	N	326	THR	CA-CB-OG1	-5.71	101.04	109.60
2	N	481	GLU	CB-CG-CD	5.70	122.30	112.60
1	F	158	LEU	CB-CA-C	5.69	121.15	110.63
1	C	158	LEU	CB-CA-C	5.68	121.14	110.63
1	B	81	ASP	CA-CB-CG	-5.68	106.92	112.60
2	O	428	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	D	100	ASP	CA-CB-CG	-5.64	106.96	112.60
2	Q	497	ASN	CA-C-N	5.64	125.49	119.28
2	Q	497	ASN	C-N-CA	5.64	125.49	119.28
1	A	5	LEU	O-C-N	5.64	127.75	121.43
1	D	38	ARG	CD-NE-CZ	-5.64	116.51	124.40
1	C	131	PHE	CA-CB-CG	5.63	119.43	113.80
2	Q	489	CYS	CA-C-O	5.63	123.80	119.46
2	R	512	ASN	CA-CB-CG	-5.63	106.97	112.60
2	M	382	GLY	CA-C-O	5.62	126.64	120.97
1	E	22	ALA	CA-C-N	5.62	128.12	120.54
1	E	22	ALA	C-N-CA	5.62	128.12	120.54
1	C	181	THR	N-CA-CB	5.61	118.36	109.71
1	F	162	GLU	N-CA-CB	5.61	118.35	109.82
1	B	166	ARG	CD-NE-CZ	5.61	132.25	124.40
1	E	129	SER	CA-C-O	-5.60	114.31	120.36
2	Q	533	THR	CA-CB-OG1	-5.60	101.20	109.60
1	B	28	ASN	O-C-N	5.60	126.11	121.35
1	F	52	LEU	CB-CA-C	5.60	121.86	109.94
1	A	189	ILE	O-C-N	5.59	128.12	121.80
1	B	38	ARG	CD-NE-CZ	5.59	132.23	124.40
2	P	359	HIS	CA-CB-CG	-5.59	108.21	113.80
1	C	178	ASP	CA-CB-CG	-5.58	107.02	112.60
2	R	367	PHE	CA-C-O	-5.58	111.31	120.80
1	E	140	HIS	CB-CA-C	-5.58	100.11	109.48
2	O	334	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	F	177	VAL	CB-CA-C	5.57	117.27	111.09
1	F	64	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	F	94	ARG	NE-CZ-NH2	-5.56	114.19	119.20
2	R	440	ARG	NH1-CZ-NH2	5.55	126.52	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	LEU	N-CA-CB	-5.55	101.82	110.98
2	N	475	ILE	N-CA-CB	5.55	119.07	111.41
1	C	100	ASP	CA-CB-CG	-5.54	107.06	112.60
2	M	306	SER	N-CA-C	5.53	118.65	110.46
2	O	417	ALA	N-CA-C	-5.52	102.82	109.83
2	N	440	ARG	CB-CA-C	5.51	118.96	110.14
2	N	494	SER	N-CA-C	-5.51	105.38	111.71
2	O	367	PHE	CA-C-O	-5.51	111.43	120.80
1	E	181	THR	O-C-N	5.50	129.89	122.96
1	F	155	CYS	O-C-N	5.50	125.76	121.47
1	D	52	LEU	CB-CA-C	5.49	122.25	110.45
2	M	514	ASN	O-C-N	5.49	126.35	121.19
2	M	533	THR	N-CA-C	-5.49	102.77	110.50
2	P	385	VAL	CA-C-O	-5.47	115.92	121.67
2	O	496	ALA	CA-C-O	-5.47	114.76	120.55
2	Q	357	GLY	N-CA-C	-5.46	105.28	112.82
2	R	410	HIS	CA-C-N	5.46	129.87	121.19
2	R	410	HIS	C-N-CA	5.46	129.87	121.19
1	F	47	GLU	CB-CG-CD	5.45	121.86	112.60
1	E	90	ASN	CA-CB-CG	5.45	118.05	112.60
1	E	38	ARG	CD-NE-CZ	-5.45	116.78	124.40
2	M	316	HIS	O-C-N	5.44	127.37	121.60
1	D	13	ALA	O-C-N	5.43	128.95	122.27
1	F	106	LEU	N-CA-CB	-5.43	101.43	111.53
1	E	198	PHE	CA-CB-CG	5.43	119.23	113.80
1	E	158	LEU	CB-CA-C	5.42	119.79	110.79
2	N	314	ASN	N-CA-CB	5.42	118.50	110.53
1	B	99	PHE	N-CA-C	-5.41	106.38	112.87
2	P	442	ILE	CB-CA-C	5.41	119.15	110.82
1	B	140	HIS	N-CA-CB	5.41	119.24	110.43
1	C	188	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	F	21	LEU	N-CA-CB	-5.41	102.06	110.98
2	M	479	TYR	CA-C-O	-5.40	115.14	121.46
2	P	457	ARG	CA-CB-CG	5.40	124.89	114.10
1	B	155	CYS	O-C-N	5.39	126.00	121.31
2	O	353	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	E	141	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	21	LEU	N-CA-C	5.38	120.51	113.30
1	A	187	ILE	O-C-N	5.38	129.07	123.26
2	O	509	ASP	CA-C-N	5.38	128.02	120.28
2	O	509	ASP	C-N-CA	5.38	128.02	120.28
2	M	387	GLN	OE1-CD-NE2	5.38	127.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ASN	CA-CB-CG	-5.37	107.23	112.60
2	P	367	PHE	CA-C-O	-5.37	111.68	120.80
1	B	184	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	B	178	ASP	CB-CA-C	5.35	119.03	111.86
2	P	514	ASN	CA-CB-CG	5.35	117.95	112.60
1	E	106	LEU	N-CA-CB	-5.33	101.47	111.13
2	P	446	PRO	N-CA-C	-5.33	103.76	111.22
2	M	442	ILE	CB-CA-C	5.33	119.53	110.95
1	E	125	HIS	CA-CB-CG	-5.32	108.48	113.80
1	D	177	VAL	CB-CA-C	5.32	117.60	110.42
2	Q	428	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	F	23	LEU	CB-CA-C	5.32	119.32	110.81
2	N	489	CYS	N-CA-C	5.32	117.29	109.42
2	N	415	TYR	CB-CA-C	5.30	118.52	109.72
1	A	192	GLU	CA-CB-CG	5.30	124.69	114.10
2	P	483	ASP	CA-C-O	5.29	124.70	119.51
2	Q	372	LEU	N-CA-C	-5.29	102.84	110.40
2	M	314	ASN	N-CA-C	-5.29	107.00	113.50
2	R	411	LYS	CB-CA-C	-5.29	102.07	110.84
1	A	52	LEU	CB-CA-C	5.28	121.19	109.94
1	C	64	ARG	CD-NE-CZ	-5.28	117.01	124.40
2	N	357	GLY	CA-C-N	5.27	127.87	120.28
2	N	357	GLY	C-N-CA	5.27	127.87	120.28
1	C	52	LEU	CB-CA-C	5.27	121.78	110.45
2	Q	514	ASN	CB-CA-C	5.27	115.39	110.17
2	Q	411	LYS	CB-CA-C	-5.26	102.10	110.84
2	Q	377	ARG	NE-CZ-NH2	5.26	123.94	119.20
2	O	392	VAL	O-C-N	5.26	127.10	121.10
2	M	463	PHE	O-C-N	5.26	129.71	123.24
2	N	324	TYR	CA-C-N	5.26	128.71	120.82
2	N	324	TYR	C-N-CA	5.26	128.71	120.82
2	P	322	PRO	CB-CA-C	5.25	121.04	112.26
2	N	529	GLY	CA-C-O	5.25	126.03	121.41
1	F	115	ASN	CA-CB-CG	5.25	117.85	112.60
2	R	505	ILE	N-CA-C	5.25	115.34	107.51
1	B	11	GLN	N-CA-CB	5.25	120.82	111.69
1	D	9	PRO	CB-CA-C	-5.25	104.23	111.21
2	Q	333	ARG	CB-CA-C	5.25	117.89	109.07
1	F	140	HIS	CB-CA-C	-5.24	101.10	109.75
2	Q	428	ARG	CD-NE-CZ	5.24	131.73	124.40
2	P	395	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	177	VAL	O-C-N	5.22	128.61	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	505	ILE	N-CA-C	5.22	115.28	107.51
1	F	30	THR	CA-CB-OG1	-5.22	101.77	109.60
1	D	3	GLU	CA-C-O	-5.21	115.07	120.70
2	Q	428	ARG	N-CA-CB	5.21	119.36	110.50
1	B	21	LEU	N-CA-CB	-5.21	103.04	110.80
2	N	367	PHE	CA-C-O	-5.21	111.95	120.80
2	O	440	ARG	O-C-N	5.21	129.40	123.31
2	P	497	ASN	CA-C-N	5.21	125.01	119.28
2	P	497	ASN	C-N-CA	5.21	125.01	119.28
2	Q	314	ASN	N-CA-C	-5.21	107.10	113.50
2	N	316	HIS	CA-CB-CG	-5.19	108.61	113.80
1	B	31	ARG	CD-NE-CZ	5.19	131.66	124.40
2	P	333	ARG	CB-CA-C	5.18	118.72	109.29
2	R	514	ASN	CA-CB-CG	5.18	117.78	112.60
2	M	339	ILE	O-C-N	5.18	127.00	121.10
1	E	5	LEU	O-C-N	5.16	127.21	121.53
2	P	321	THR	N-CA-CB	-5.16	104.69	111.09
2	P	454	ASN	CA-CB-CG	5.16	117.75	112.60
2	M	357	GLY	N-CA-C	-5.15	105.71	112.82
2	N	338	SER	O-C-N	5.15	129.07	123.04
2	N	439	PHE	CA-C-N	-5.15	115.51	122.77
2	N	439	PHE	C-N-CA	-5.15	115.51	122.77
2	N	428	ARG	CB-CG-CD	5.15	123.14	111.30
1	C	64	ARG	CA-C-O	-5.15	113.65	119.78
1	E	116	ASN	N-CA-C	-5.15	103.25	110.35
2	R	392	VAL	O-C-N	5.15	126.97	121.10
1	E	4	LEU	CA-C-O	-5.13	115.21	121.88
2	R	307	ARG	CA-C-O	-5.13	115.11	121.11
1	C	28	ASN	O-C-N	5.12	126.21	121.80
1	F	100	ASP	CA-CB-CG	-5.12	107.48	112.60
1	B	163	GLN	CA-C-O	5.12	122.62	119.29
1	A	165	GLN	OE1-CD-NE2	-5.11	117.49	122.60
2	Q	457	ARG	NE-CZ-NH2	-5.11	114.60	119.20
2	R	457	ARG	N-CA-CB	5.11	117.34	110.14
1	F	181	THR	N-CA-CB	5.10	117.56	109.71
1	C	48	HIS	CA-CB-CG	-5.09	108.70	113.80
1	C	150	GLN	N-CA-CB	5.09	117.56	109.82
2	M	367	PHE	CA-C-O	-5.08	112.16	120.80
1	C	5	LEU	O-C-N	5.07	127.11	121.43
1	F	97	THR	N-CA-CB	5.07	118.44	110.23
2	R	307	ARG	N-CA-C	-5.07	101.49	109.50
2	M	434	ASP	CA-CB-CG	-5.06	107.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	350	ASN	CA-CB-CG	-5.06	107.54	112.60
1	B	183	TYR	N-CA-CB	5.05	119.54	110.80
2	M	322	PRO	CA-C-O	-5.05	111.41	120.60
2	P	533	THR	CA-CB-OG1	-5.04	102.03	109.60
1	E	99	PHE	N-CA-C	-5.04	106.39	112.54
1	F	178	ASP	N-CA-C	-5.04	104.46	111.52
2	Q	441	THR	N-CA-CB	-5.04	101.79	110.76
1	F	38	ARG	CB-CA-C	5.03	119.68	111.23
1	A	165	GLN	CB-CG-CD	5.03	121.15	112.60
2	P	442	ILE	CA-CB-CG2	5.03	119.05	110.50
1	F	139	LEU	CA-C-N	5.02	129.65	122.72
1	F	139	LEU	C-N-CA	5.02	129.65	122.72
1	F	176	GLU	CB-CG-CD	5.02	121.13	112.60
2	R	440	ARG	CB-CG-CD	-5.02	99.75	111.30
2	M	449	TRP	O-C-N	5.02	129.00	123.33
1	E	11	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	B	171	ILE	N-CA-C	5.01	114.98	107.51
2	Q	457	ARG	NE-CZ-NH1	5.01	126.51	121.50
1	F	94	ARG	CD-NE-CZ	5.01	131.42	124.40
2	O	383	ARG	CD-NE-CZ	-5.01	117.39	124.40
2	N	457	ARG	NE-CZ-NH2	-5.01	114.69	119.20
2	O	383	ARG	NE-CZ-NH2	-5.00	114.70	119.20
2	O	457	ARG	CD-NE-CZ	5.00	131.41	124.40
1	E	81	ASP	N-CA-C	5.00	118.54	112.23
2	O	495	ILE	CA-C-N	5.00	126.99	120.28
2	O	495	ILE	C-N-CA	5.00	126.99	120.28
2	P	484	PRO	CA-C-N	5.00	127.92	120.31
2	P	484	PRO	C-N-CA	5.00	127.92	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	184	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	45	0
1	B	1571	0	1499	45	0
1	C	1571	0	1499	52	0
1	D	1571	0	1499	52	0
1	E	1571	0	1499	53	0
1	F	1571	0	1499	66	0
2	M	1844	0	1796	64	0
2	N	1844	0	1796	31	0
2	O	1844	0	1796	55	0
2	P	1844	0	1796	51	0
2	Q	1844	0	1796	54	0
2	R	1844	0	1796	65	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	20	0	10	3	0
4	N	20	0	10	1	0
4	O	20	0	9	2	0
4	P	20	0	9	2	0
4	Q	20	0	10	3	0
4	R	20	0	10	3	0
5	A	83	0	0	0	0
5	B	79	0	0	1	0
5	C	81	0	0	1	0
5	D	81	0	0	2	0
5	E	84	0	0	1	0
5	F	80	0	0	3	0
5	M	151	0	0	5	0
5	N	161	0	0	3	0
5	O	155	0	0	3	0
5	P	152	0	0	3	0
5	Q	153	0	0	6	0
5	R	156	0	0	5	0
All	All	22032	0	19828	591	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (591) 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:E:165:GLN:H	1:E:165:GLN:NE2	1.26	1.33
1:E:165:GLN:HE21	1:E:165:GLN:N	1.27	1.31
1:F:64:ARG:NH1	1:F:100:ASP:O	1.84	1.10
1:D:64:ARG:NH1	1:D:100:ASP:O	1.85	1.09
2:R:447:TYR:OH	4:R:550:3HB:H4	1.55	1.06
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.39	1.01
1:F:165:GLN:H	1:F:165:GLN:NE2	1.59	1.01
1:B:165:GLN:H	1:B:165:GLN:NE2	1.56	1.01
2:N:447:TYR:OH	4:N:550:3HB:H4	1.60	1.00
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.42	1.00
1:A:98:THR:HB	1:A:100:ASP:OD1	1.60	0.99
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.43	0.99
1:D:98:THR:OG1	1:D:102:GLY:N	1.95	0.98
1:C:64:ARG:NH1	1:C:100:ASP:O	1.98	0.96
2:R:361:HIS:H	2:R:361:HIS:CD2	1.81	0.93
1:D:165:GLN:H	1:D:165:GLN:HE21	1.11	0.93
2:M:390:LYS:HD2	5:M:640:HOH:O	1.70	0.92
2:R:497:ASN:ND2	2:R:499:GLU:H	1.68	0.91
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.84	0.91
1:E:64:ARG:HG2	1:E:64:ARG:HH11	1.33	0.91
1:E:98:THR:OG1	1:E:102:GLY:N	2.03	0.91
1:D:165:GLN:H	1:D:165:GLN:NE2	1.67	0.90
1:B:165:GLN:H	1:B:165:GLN:HE21	0.91	0.90
1:A:64:ARG:NH1	1:A:100:ASP:O	2.05	0.89
1:C:98:THR:OG1	1:C:102:GLY:N	2.05	0.88
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.04	0.88
1:F:98:THR:OG1	1:F:102:GLY:N	2.04	0.87
1:B:165:GLN:HE21	1:B:165:GLN:N	1.71	0.87
2:R:361:HIS:H	2:R:361:HIS:HD2	1.18	0.87
1:A:98:THR:OG1	1:A:102:GLY:N	2.06	0.87
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.57	0.87
2:R:497:ASN:HD22	2:R:499:GLU:H	1.20	0.87
1:E:64:ARG:HG2	1:E:64:ARG:NH1	1.91	0.85
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.92	0.85
2:M:447:TYR:OH	4:M:550:3HB:H4	1.77	0.84
1:C:98:THR:HB	1:C:100:ASP:OD1	1.78	0.83
1:E:64:ARG:NH1	1:E:100:ASP:O	2.11	0.82
1:C:165:GLN:NE2	1:C:165:GLN:H	1.77	0.82
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.61	0.82
1:D:98:THR:HB	1:D:100:ASP:OD1	1.78	0.82
1:E:98:THR:HB	1:E:100:ASP:OD1	1.79	0.82
2:M:361:HIS:H	2:M:361:HIS:CD2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:HH12	1:D:100:ASP:C	1.89	0.80
1:C:18:HIS:ND1	5:C:280:HOH:O	2.09	0.80
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.64	0.80
1:B:176:GLU:HG3	1:B:180:LYS:O	1.82	0.80
1:B:98:THR:HB	1:B:100:ASP:OD1	1.81	0.80
2:P:361:HIS:H	2:P:361:HIS:CD2	2.01	0.79
2:O:361:HIS:H	2:O:361:HIS:CD2	2.02	0.77
2:O:497:ASN:HD22	2:O:499:GLU:H	1.32	0.77
2:O:390:LYS:HD2	5:O:650:HOH:O	1.85	0.77
1:F:98:THR:HB	1:F:100:ASP:OD1	1.85	0.76
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.49	0.76
2:Q:390:LYS:HD2	5:Q:1020:HOH:O	1.84	0.76
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.50	0.76
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.68	0.76
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.04	0.75
1:B:18:HIS:ND1	5:B:470:HOH:O	2.18	0.75
1:E:180:LYS:HG3	1:E:181:THR:N	1.99	0.74
2:Q:447:TYR:OH	4:Q:550:3HB:H4	1.86	0.74
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.69	0.74
2:P:447:TYR:OH	4:P:550:3HB:H4	1.85	0.74
2:M:361:HIS:H	2:M:361:HIS:HD2	1.36	0.74
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.88	0.73
1:A:78:GLU:HG2	2:M:301:PRO:HB2	1.70	0.73
1:D:18:HIS:ND1	5:D:942:HOH:O	2.20	0.73
2:O:497:ASN:ND2	2:O:499:GLU:H	1.87	0.73
2:R:324:TYR:OH	4:R:550:3HB:O1'	2.04	0.72
1:D:165:GLN:HE21	1:D:165:GLN:N	1.87	0.72
1:B:3:GLU:HA	1:B:3:GLU:OE1	1.89	0.72
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.72	0.72
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.54	0.72
2:Q:522:ARG:NH1	5:Q:1058:HOH:O	2.22	0.72
1:B:98:THR:OG1	1:B:102:GLY:N	2.22	0.72
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.53	0.71
2:M:497:ASN:ND2	2:M:499:GLU:H	1.86	0.71
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.56	0.71
2:P:361:HIS:H	2:P:361:HIS:HD2	1.37	0.71
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.25	0.71
2:N:390:LYS:HD3	5:N:649:HOH:O	1.91	0.70
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.72	0.70
1:C:177:VAL:O	1:C:180:LYS:HB3	1.92	0.70
1:A:176:GLU:HG3	1:A:180:LYS:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:H	1:F:165:GLN:HE21	1.41	0.69
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.74	0.69
2:P:313:ARG:O	2:P:318:LYS:HE3	1.91	0.69
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.11	0.69
1:F:100:ASP:OD1	1:F:100:ASP:N	2.24	0.69
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.75	0.69
2:R:536:GLU:HB2	5:R:1337:HOH:O	1.92	0.69
1:D:100:ASP:CG	1:D:101:ALA:H	2.01	0.68
2:O:390:LYS:HD3	5:O:729:HOH:O	1.93	0.68
1:E:18:HIS:ND1	5:E:282:HOH:O	2.27	0.68
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.41	0.68
2:Q:324:TYR:OH	4:Q:550:3HB:O1'	2.07	0.68
1:D:177:VAL:O	1:D:180:LYS:HB3	1.94	0.67
1:C:99:PHE:CE2	2:O:411:LYS:HD2	2.29	0.67
2:R:361:HIS:CD2	2:R:361:HIS:N	2.54	0.67
2:Q:376:GLU:OE1	5:Q:1008:HOH:O	2.11	0.67
1:C:165:GLN:H	1:C:165:GLN:CD	2.00	0.67
2:O:361:HIS:H	2:O:361:HIS:HD2	1.44	0.66
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.77	0.66
1:C:100:ASP:OD1	1:C:100:ASP:N	2.29	0.66
1:A:100:ASP:CG	1:A:101:ALA:H	2.03	0.66
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.42	0.66
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.94	0.66
2:M:390:LYS:HD3	5:M:716:HOH:O	1.96	0.65
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.31	0.65
2:R:307:ARG:CG	2:R:533:THR:HG22	2.26	0.65
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.62	0.65
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.30	0.65
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.96	0.65
2:N:361:HIS:CD2	2:N:361:HIS:H	2.15	0.65
2:N:497:ASN:HD22	2:N:499:GLU:H	1.45	0.65
1:B:64:ARG:NH1	1:B:100:ASP:O	2.30	0.64
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.62	0.64
1:E:98:THR:O	1:E:102:GLY:HA2	1.96	0.64
1:F:147:ASP:OD2	1:F:174:ARG:HD2	1.97	0.64
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.98	0.64
1:A:165:GLN:CD	1:A:165:GLN:H	2.06	0.63
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.28	0.63
2:N:478:LEU:C	2:N:478:LEU:HD23	2.22	0.63
2:M:497:ASN:HD22	2:M:499:GLU:H	1.43	0.63
1:B:52:LEU:C	1:B:52:LEU:HD22	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:376:GLU:OE1	5:P:645:HOH:O	2.15	0.63
1:F:49:ILE:HA	1:F:180:LYS:HE3	1.80	0.63
2:R:497:ASN:HD22	2:R:497:ASN:C	2.05	0.63
1:C:3:GLU:OE1	1:C:3:GLU:HA	1.99	0.62
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.14	0.62
2:Q:411:LYS:O	2:Q:414:ARG:NH1	2.32	0.62
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.64	0.62
2:P:497:ASN:ND2	2:P:499:GLU:H	1.96	0.62
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.07	0.62
1:E:100:ASP:CG	1:E:101:ALA:H	2.07	0.62
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.13	0.62
1:D:64:ARG:NH1	1:D:64:ARG:HG2	2.14	0.62
2:P:414:ARG:NE	2:P:414:ARG:HA	2.14	0.62
2:O:447:TYR:OH	4:O:550:3HB:H4	2.00	0.62
1:F:177:VAL:O	1:F:180:LYS:HB3	2.00	0.62
2:P:497:ASN:HD22	2:P:499:GLU:H	1.47	0.62
1:C:131:PHE:O	1:C:132:ALA:HB2	2.00	0.61
2:N:390:LYS:HE2	5:N:730:HOH:O	1.99	0.61
1:E:64:ARG:HH12	1:E:100:ASP:C	2.05	0.60
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.66	0.60
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.65	0.60
2:R:411:LYS:O	2:R:414:ARG:NH1	2.34	0.60
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.01	0.60
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.65	0.60
1:F:165:GLN:H	1:F:165:GLN:CD	2.09	0.60
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.31	0.60
1:F:100:ASP:CG	1:F:101:ALA:H	2.09	0.60
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.00	0.60
1:E:64:ARG:HH11	1:E:64:ARG:CG	1.98	0.59
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.17	0.59
2:P:376:GLU:O	2:P:442:ILE:HA	2.03	0.59
2:M:354:LEU:HD23	2:M:356:PHE:CE1	2.37	0.59
2:Q:536:GLU:HB2	5:Q:1101:HOH:O	2.01	0.59
2:Q:465:ILE:HD12	2:Q:465:ILE:N	2.17	0.59
2:M:536:GLU:HB2	5:M:695:HOH:O	2.03	0.59
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.84	0.59
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.37	0.59
2:R:390:LYS:HD2	5:R:1256:HOH:O	2.01	0.59
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.82	0.59
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.49	0.59
2:R:405:GLY:HA3	5:R:1260:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:O	2:N:426:VAL:HG21	2.03	0.58
2:R:497:ASN:ND2	2:R:499:GLU:N	2.47	0.58
2:R:390:LYS:HD3	5:R:1374:HOH:O	2.03	0.58
1:B:176:GLU:HG3	1:B:180:LYS:C	2.29	0.58
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.52	0.58
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.00	0.58
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.86	0.58
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.19	0.58
1:D:19:ILE:O	2:P:426:VAL:HG21	2.02	0.58
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.85	0.58
2:R:399:MET:HA	2:R:462:HIS:O	2.03	0.58
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.85	0.58
2:P:405:GLY:HA3	5:P:653:HOH:O	2.03	0.58
1:C:100:ASP:CG	1:C:101:ALA:H	2.10	0.58
2:R:356:PHE:HD1	2:R:428:ARG:HD3	1.68	0.58
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.51	0.57
2:M:416:LEU:C	2:M:416:LEU:HD23	2.29	0.57
2:N:497:ASN:ND2	2:N:499:GLU:H	2.03	0.57
1:F:98:THR:O	1:F:102:GLY:HA2	2.03	0.57
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.03	0.57
2:Q:361:HIS:CG	2:Q:429:CME:HE3	2.40	0.57
2:R:497:ASN:HD22	2:R:499:GLU:N	1.96	0.57
2:P:489:CYS:O	2:P:493:LYS:HG3	2.04	0.57
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.01	0.57
1:A:176:GLU:HA	1:A:180:LYS:O	2.05	0.57
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.86	0.57
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.26	0.57
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.85	0.57
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.19	0.57
2:P:411:LYS:O	2:P:414:ARG:NH1	2.37	0.57
2:N:313:ARG:O	2:N:318:LYS:HE2	2.05	0.56
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.38	0.56
1:B:50:LEU:O	1:B:182:ALA:HA	2.05	0.56
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.04	0.56
1:A:50:LEU:O	1:A:182:ALA:HA	2.04	0.56
2:M:478:LEU:HD23	2:M:478:LEU:C	2.29	0.56
2:O:497:ASN:HD22	2:O:497:ASN:C	2.13	0.56
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.20	0.56
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.35	0.56
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.86	0.56
1:F:19:ILE:O	2:R:426:VAL:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.53	0.56
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.03	0.56
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.94	0.56
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.41	0.56
2:O:376:GLU:O	2:O:442:ILE:HA	2.05	0.56
2:M:305:ASN:O	2:M:533:THR:HG23	2.06	0.55
1:B:143:LEU:C	1:B:143:LEU:HD23	2.31	0.55
2:M:324:TYR:OH	4:M:550:3HB:O1'	2.10	0.55
1:F:36:TRP:CG	1:F:37:ASN:H	2.25	0.55
1:F:176:GLU:OE2	1:F:179:GLY:C	2.50	0.55
1:D:18:HIS:CG	5:D:942:HOH:O	2.59	0.55
2:M:497:ASN:HD22	2:M:498:PRO:N	2.05	0.55
2:N:359:HIS:O	2:N:366:ASN:HB3	2.07	0.55
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.04	0.55
2:M:522:ARG:NH1	5:M:662:HOH:O	2.39	0.54
2:P:484:PRO:O	2:P:488:MET:HE3	2.07	0.54
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.42	0.54
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.53	0.54
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.73	0.54
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.33	0.54
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.42	0.54
1:C:41:LYS:NZ	1:C:86:GLU:O	2.31	0.54
1:E:133:ARG:HG3	2:Q:326:THR:HG21	1.90	0.54
1:E:143:LEU:HD23	1:E:143:LEU:C	2.33	0.54
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.89	0.54
2:P:497:ASN:HD22	2:P:497:ASN:C	2.15	0.54
2:Q:405:GLY:HA3	5:Q:1024:HOH:O	2.07	0.54
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.73	0.54
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.89	0.54
2:P:522:ARG:NH1	5:P:673:HOH:O	2.38	0.54
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.90	0.54
2:M:399:MET:HE2	2:M:461:ILE:HG21	1.89	0.53
2:R:361:HIS:CG	2:R:429:CME:HE3	2.43	0.53
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.43	0.53
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.36	0.53
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.38	0.53
2:O:522:ARG:NH1	5:O:674:HOH:O	2.39	0.53
2:Q:447:TYR:HE1	4:Q:550:3HB:H5	1.73	0.53
2:M:361:HIS:CG	2:M:429:CME:HE3	2.44	0.53
1:D:64:ARG:CZ	1:D:100:ASP:O	2.55	0.53
2:M:497:ASN:HD22	2:M:497:ASN:C	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:O	1:B:102:GLY:HA2	2.10	0.52
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.45	0.52
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.92	0.52
2:O:361:HIS:CG	2:O:429:CME:HE3	2.44	0.52
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.35	0.52
1:D:64:ARG:HH11	1:D:64:ARG:CG	2.22	0.52
2:P:359:HIS:O	2:P:366:ASN:HB3	2.09	0.52
1:D:52:LEU:C	1:D:52:LEU:HD22	2.35	0.52
2:M:361:HIS:ND1	2:M:429:CME:HE3	2.25	0.52
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.25	0.52
1:C:165:GLN:NE2	1:C:165:GLN:N	2.55	0.52
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.92	0.52
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.25	0.52
1:A:78:GLU:CG	2:M:301:PRO:CB	2.85	0.52
2:Q:488:MET:HE2	1:F:1:PRO:HG2	1.92	0.52
1:F:155:CYS:O	1:F:159:ASN:ND2	2.43	0.51
2:R:400:TRP:HA	2:R:425:GLY:O	2.10	0.51
2:O:410:HIS:CE1	2:O:412:ASN:H	2.29	0.51
2:O:478:LEU:HD23	2:O:478:LEU:C	2.36	0.51
2:M:359:HIS:O	2:M:366:ASN:HB3	2.10	0.51
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.73	0.51
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.40	0.51
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.10	0.51
1:D:155:CYS:HB3	1:D:158:LEU:HB2	1.92	0.51
2:R:306:SER:CB	2:R:530:GLN:HE21	2.22	0.51
2:R:497:ASN:HD22	2:R:498:PRO:N	2.08	0.51
1:B:100:ASP:OD1	1:B:100:ASP:N	2.42	0.51
2:N:361:HIS:H	2:N:361:HIS:HD2	1.58	0.51
2:P:497:ASN:HD22	2:P:498:PRO:N	2.09	0.51
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.11	0.51
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.26	0.51
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.76	0.51
1:C:143:LEU:HD23	1:C:143:LEU:C	2.36	0.51
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.25	0.50
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.93	0.50
2:N:307:ARG:CG	2:N:533:THR:HG22	2.38	0.50
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.44	0.50
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.27	0.50
1:E:39:LEU:CD1	1:E:106:LEU:HD11	2.42	0.50
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.94	0.50
1:D:100:ASP:OD1	1:D:100:ASP:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.93	0.50
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.11	0.50
1:F:131:PHE:O	1:F:132:ALA:HB2	2.12	0.50
1:C:98:THR:O	1:C:102:GLY:HA2	2.10	0.50
2:N:414:ARG:NE	2:N:414:ARG:HA	2.27	0.50
2:O:308:PHE:CE1	2:O:530:GLN:HB2	2.46	0.50
1:C:36:TRP:CG	1:C:37:ASN:H	2.30	0.49
2:P:410:HIS:ND1	2:P:411:LYS:N	2.60	0.49
2:M:314:ASN:OD1	2:M:318:LYS:HE2	2.11	0.49
2:M:448:PRO:HB2	2:P:516:MET:HA	1.94	0.49
1:D:18:HIS:CE1	1:D:99:PHE:HE1	2.31	0.49
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.47	0.49
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.12	0.49
1:D:100:ASP:CG	1:D:101:ALA:N	2.70	0.49
1:D:143:LEU:C	1:D:143:LEU:HD23	2.37	0.49
1:F:115:ASN:HA	1:F:121:PRO:HA	1.94	0.49
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.42	0.49
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.43	0.49
1:F:184:ARG:NH1	1:F:184:ARG:HG3	2.27	0.49
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.94	0.49
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.95	0.49
2:O:416:LEU:C	2:O:416:LEU:HD23	2.38	0.49
1:E:167:ARG:O	1:E:171:ILE:HD12	2.13	0.49
2:R:359:HIS:O	2:R:366:ASN:HB3	2.13	0.49
2:O:324:TYR:OH	4:O:550:3HB:O1'	2.09	0.48
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.28	0.48
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.95	0.48
1:D:51:LEU:O	1:D:105:THR:HA	2.13	0.48
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.28	0.48
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.28	0.48
2:M:495:ILE:HG21	2:M:500:ALA:HB3	1.95	0.48
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.95	0.48
1:B:177:VAL:O	1:B:180:LYS:HB3	2.14	0.48
2:N:399:MET:HA	2:N:462:HIS:O	2.13	0.48
1:F:143:LEU:C	1:F:143:LEU:HD23	2.37	0.48
1:A:1:PRO:HG2	2:O:488:MET:HE2	1.96	0.48
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.48	0.48
1:F:165:GLN:NE2	1:F:165:GLN:N	2.43	0.48
2:R:432:ASP:OD1	2:R:432:ASP:C	2.55	0.48
2:M:400:TRP:HA	2:M:425:GLY:O	2.13	0.48
2:O:484:PRO:O	2:O:487:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:416:LEU:HD23	2:R:417:ALA:N	2.29	0.48
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.61	0.48
2:M:448:PRO:CB	2:P:516:MET:HA	2.44	0.48
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.48	0.48
1:B:52:LEU:C	1:B:52:LEU:CD2	2.86	0.48
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.62	0.48
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.44	0.48
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.72	0.48
2:R:416:LEU:HD23	2:R:416:LEU:C	2.39	0.48
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.81	0.47
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.48	0.47
1:F:18:HIS:CG	5:F:1414:HOH:O	2.66	0.47
1:E:113:VAL:HG13	1:E:122:MET:O	2.13	0.47
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.80	0.47
2:R:372:LEU:HD12	2:R:372:LEU:HA	1.79	0.47
2:N:400:TRP:HA	2:N:425:GLY:O	2.14	0.47
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.96	0.47
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.72	0.47
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.13	0.47
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.45	0.47
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.96	0.47
2:O:361:HIS:CD2	2:O:361:HIS:N	2.74	0.47
1:D:36:TRP:CG	1:D:37:ASN:H	2.32	0.47
1:C:99:PHE:HE2	2:O:411:LYS:HD2	1.76	0.47
2:O:307:ARG:HG2	2:O:533:THR:HG22	1.95	0.47
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.49	0.47
2:P:356:PHE:HD1	2:P:428:ARG:HD3	1.79	0.47
1:E:22:ALA:O	1:E:25:ALA:HB3	2.14	0.47
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.82	0.47
1:F:64:ARG:HD3	1:F:99:PHE:O	2.15	0.47
1:A:98:THR:HB	1:A:100:ASP:CG	2.37	0.47
1:D:50:LEU:O	1:D:182:ALA:HA	2.15	0.47
1:E:6:PRO:HB2	2:Q:503:GLN:HE22	1.79	0.47
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.96	0.47
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.81	0.47
1:A:98:THR:O	1:A:102:GLY:HA2	2.15	0.46
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.96	0.46
1:C:50:LEU:O	1:C:182:ALA:HA	2.15	0.46
2:Q:429:CME:HE2	2:Q:438:SER:O	2.15	0.46
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.97	0.46
1:C:3:GLU:OE1	1:C:3:GLU:CA	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.82	0.46
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.97	0.46
2:O:410:HIS:ND1	2:O:411:LYS:N	2.64	0.46
2:R:383:ARG:HG3	2:R:436:TYR:CE1	2.50	0.46
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.28	0.46
1:D:64:ARG:NH1	1:D:100:ASP:C	2.60	0.46
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.15	0.46
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.34	0.46
1:A:64:ARG:HD3	1:A:99:PHE:O	2.16	0.46
2:P:478:LEU:C	2:P:478:LEU:HD23	2.41	0.46
2:M:307:ARG:HD2	5:M:652:HOH:O	2.16	0.46
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.49	0.46
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.51	0.46
1:A:163:GLN:OE1	1:A:165:GLN:NE2	2.44	0.46
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.34	0.46
1:A:28:ASN:HB3	1:A:29:PRO:HD2	1.97	0.46
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.81	0.46
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.98	0.46
2:Q:399:MET:HA	2:Q:462:HIS:O	2.16	0.46
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.40	0.46
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.98	0.46
1:E:164:PRO:HD2	1:E:165:GLN:HE22	1.80	0.46
1:F:38:ARG:HA	1:F:107:HIS:HB2	1.98	0.46
1:F:176:GLU:HA	1:F:180:LYS:O	2.16	0.46
1:A:6:PRO:HB2	2:M:503:GLN:HE22	1.81	0.45
2:N:361:HIS:CG	2:N:429:CME:HE3	2.51	0.45
2:N:448:PRO:HD3	2:N:456:TRP:CZ3	2.51	0.45
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.97	0.45
2:O:381:ALA:O	2:O:522:ARG:HA	2.16	0.45
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.75	0.45
2:O:304:ASP:HB2	2:O:343:ILE:HB	1.99	0.45
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	1.98	0.45
2:R:465:ILE:N	2:R:465:ILE:HD12	2.30	0.45
2:M:447:TYR:HE1	4:M:550:3HB:H5	1.82	0.45
2:O:315:TRP:CZ2	2:O:503:GLN:NE2	2.84	0.45
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.31	0.45
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.51	0.45
1:C:163:GLN:CB	1:C:165:GLN:HE22	2.26	0.45
1:E:164:PRO:N	1:E:165:GLN:NE2	2.65	0.45
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.49	0.45
1:C:155:CYS:O	1:C:159:ASN:ND2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.99	0.45
1:C:19:ILE:HD13	1:C:19:ILE:HG21	1.74	0.45
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.52	0.45
1:F:78:GLU:HB2	1:F:80:GLN:HE21	1.82	0.45
1:A:36:TRP:CG	1:A:37:ASN:H	2.34	0.45
2:O:413:ASP:C	2:O:414:ARG:HD2	2.41	0.45
1:F:98:THR:HB	1:F:100:ASP:CG	2.40	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.42	0.45
1:C:64:ARG:NH1	1:C:64:ARG:HG2	2.32	0.44
1:D:63:VAL:HG12	1:D:66:SER:HB3	1.99	0.44
1:D:180:LYS:HG3	1:D:181:THR:N	2.30	0.44
2:P:400:TRP:HA	2:P:425:GLY:O	2.17	0.44
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.87	0.44
1:C:66:SER:HA	1:C:132:ALA:HB2	1.99	0.44
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.15	0.44
2:R:505:ILE:HG22	2:R:507:LYS:HE3	1.99	0.44
1:A:165:GLN:NE2	1:A:165:GLN:H	2.15	0.44
1:F:98:THR:HG1	1:F:103:GLU:H	1.65	0.44
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.32	0.44
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.71	0.44
2:M:303:GLN:CB	2:M:305:ASN:ND2	2.81	0.44
1:F:74:ASP:HB2	5:F:1268:HOH:O	2.17	0.44
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.80	0.44
2:P:437:TYR:CD1	2:P:437:TYR:C	2.96	0.44
1:F:114:VAL:HG23	1:F:122:MET:CE	2.47	0.44
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.52	0.44
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.79	0.44
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.18	0.44
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.52	0.44
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.76	0.44
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.74	0.44
2:P:307:ARG:HA	2:P:307:ARG:HD3	1.86	0.44
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.17	0.44
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.98	0.44
1:B:18:HIS:CE1	1:B:99:PHE:HE1	2.36	0.44
2:N:360:ASP:O	2:N:427:GLY:HA2	2.18	0.44
1:C:18:HIS:CE1	1:C:99:PHE:HE1	2.35	0.44
1:C:48:HIS:HA	1:C:109:VAL:HG12	2.00	0.44
1:D:191:GLY:O	1:D:194:GLU:HB2	2.18	0.44
2:P:318:LYS:HA	2:P:318:LYS:HD3	1.55	0.44
2:P:483:ASP:HA	2:P:484:PRO:HD2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:O	2:Q:387:GLN:HG2	2.17	0.44
1:E:8:THR:HA	1:E:9:PRO:HD3	1.85	0.44
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.80	0.44
1:C:64:ARG:HG2	1:C:64:ARG:HH11	1.83	0.43
1:E:52:LEU:HA	1:E:104:TRP:O	2.18	0.43
2:R:410:HIS:ND1	2:R:411:LYS:N	2.66	0.43
2:N:488:MET:HE2	1:C:1:PRO:HG2	1.99	0.43
1:C:4:LEU:HB3	2:O:387:GLN:HB3	2.00	0.43
1:C:52:LEU:C	1:C:52:LEU:HD22	2.42	0.43
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.52	0.43
1:D:98:THR:HB	1:D:100:ASP:CG	2.42	0.43
1:E:36:TRP:CG	1:E:37:ASN:H	2.36	0.43
2:P:447:TYR:HB2	2:P:448:PRO:HD2	2.00	0.43
2:R:437:TYR:CD1	2:R:437:TYR:C	2.96	0.43
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.74	0.43
1:B:8:THR:HA	1:B:9:PRO:HD3	1.89	0.43
1:B:36:TRP:CG	1:B:37:ASN:H	2.36	0.43
2:O:472:THR:HG22	2:O:528:ARG:HB2	2.00	0.43
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.53	0.43
2:P:324:TYR:OH	4:P:550:3HB:O1'	2.11	0.43
2:Q:497:ASN:HD22	2:Q:498:PRO:CD	2.32	0.43
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.53	0.43
1:F:19:ILE:HD13	1:F:19:ILE:HG21	1.79	0.43
1:F:41:LYS:HD2	1:F:88:ALA:HA	2.01	0.43
1:F:50:LEU:O	1:F:182:ALA:HA	2.19	0.43
2:R:431:THR:HG22	2:R:437:TYR:HB3	1.98	0.43
1:C:70:VAL:HG11	1:C:106:LEU:CD2	2.49	0.43
1:D:155:CYS:O	1:D:159:ASN:ND2	2.51	0.43
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.83	0.43
1:F:52:LEU:O	1:F:184:ARG:HA	2.18	0.43
2:M:416:LEU:C	2:M:416:LEU:CD2	2.91	0.43
2:P:326:THR:HG22	2:P:330:ARG:HD2	2.01	0.43
1:E:53:GLY:O	1:E:103:GLU:HG3	2.19	0.43
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.44	0.43
2:R:447:TYR:HE1	4:R:550:3HB:H5	1.82	0.43
1:B:147:ASP:OD2	1:B:183:TYR:OH	2.31	0.43
2:O:497:ASN:HD22	2:O:498:PRO:N	2.16	0.43
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.80	0.43
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.49	0.43
2:N:361:HIS:CD2	5:N:709:HOH:O	2.72	0.43
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:HG21	1:D:92:PHE:CE2	2.52	0.42
1:E:70:VAL:HG12	1:E:128:ILE:HG12	2.00	0.42
2:R:415:TYR:CE1	2:R:416:LEU:CD2	3.02	0.42
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.54	0.42
2:Q:486:ILE:N	2:Q:487:PRO:HD2	2.33	0.42
1:F:52:LEU:C	1:F:52:LEU:HD22	2.43	0.42
2:R:536:GLU:HG3	5:R:1229:HOH:O	2.18	0.42
2:Q:362:ASP:OD1	2:Q:364:LEU:HB2	2.19	0.42
2:Q:497:ASN:C	2:Q:497:ASN:ND2	2.76	0.42
2:R:361:HIS:ND1	2:R:429:CME:HE3	2.34	0.42
1:A:180:LYS:HG2	1:A:181:THR:N	2.33	0.42
1:B:165:GLN:NE2	1:B:165:GLN:N	2.41	0.42
1:C:99:PHE:CD2	2:O:411:LYS:HD2	2.54	0.42
1:F:165:GLN:HE21	1:F:165:GLN:N	2.11	0.42
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.62	0.42
2:R:413:ASP:C	2:R:414:ARG:HD2	2.45	0.42
1:C:191:GLY:O	1:C:194:GLU:HB2	2.19	0.42
1:D:52:LEU:HA	1:D:104:TRP:O	2.19	0.42
1:E:100:ASP:OD1	1:E:100:ASP:N	2.38	0.42
1:E:176:GLU:HA	1:E:180:LYS:O	2.19	0.42
2:R:341:GLN:HB3	2:R:346:THR:CG2	2.50	0.42
1:C:168:GLU:HA	1:C:171:ILE:HD12	2.01	0.42
1:F:69:GLU:OE2	1:F:94:ARG:HD3	2.19	0.42
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.93	0.42
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.55	0.42
1:B:176:GLU:HA	1:B:180:LYS:O	2.20	0.42
1:D:98:THR:O	1:D:102:GLY:HA2	2.20	0.42
1:F:18:HIS:ND1	5:F:1414:HOH:O	2.37	0.42
2:R:306:SER:OG	2:R:530:GLN:NE2	2.49	0.42
2:R:468:PRO:HD2	2:R:472:THR:HG21	2.02	0.42
2:M:376:GLU:O	2:M:442:ILE:HA	2.20	0.42
2:M:447:TYR:HB2	2:M:448:PRO:HD2	2.02	0.42
1:B:161:ILE:HD13	1:B:196:VAL:HG21	2.02	0.42
2:N:376:GLU:O	2:N:442:ILE:HA	2.20	0.42
2:O:410:HIS:CE1	2:O:411:LYS:HG3	2.55	0.42
1:F:36:TRP:CG	1:F:37:ASN:N	2.88	0.42
1:F:47:GLU:O	1:F:49:ILE:HG23	2.20	0.42
1:A:78:GLU:HB3	1:A:80:GLN:HE21	1.85	0.41
1:E:70:VAL:HG21	1:E:106:LEU:HD21	2.03	0.41
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.53	0.41
2:P:381:ALA:O	2:P:522:ARG:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:307:ARG:HG2	2:R:533:THR:CG2	2.49	0.41
1:A:19:ILE:HG21	2:M:410:HIS:HB2	2.02	0.41
2:R:363:LEU:N	2:R:363:LEU:HD12	2.36	0.41
1:A:49:ILE:C	1:A:180:LYS:HE2	2.46	0.41
2:M:385:VAL:O	2:M:526:VAL:HA	2.20	0.41
2:P:383:ARG:NH2	2:P:391:PRO:HG3	2.35	0.41
2:Q:390:LYS:HE2	5:Q:1138:HOH:O	2.21	0.41
2:N:497:ASN:HD22	2:N:497:ASN:C	2.28	0.41
2:O:364:LEU:HD11	2:O:442:ILE:HG23	2.03	0.41
2:P:399:MET:HA	2:P:462:HIS:O	2.21	0.41
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.35	0.41
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.80	0.41
1:F:8:THR:HA	1:F:9:PRO:HD3	1.87	0.41
1:B:162:GLU:O	1:B:164:PRO:HD3	2.21	0.41
2:N:420:ASP:HA	2:N:421:PRO:HD2	1.94	0.41
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.83	0.41
1:E:165:GLN:NE2	1:E:165:GLN:N	2.11	0.41
2:Q:361:HIS:ND1	2:Q:429:CME:HE3	2.36	0.41
1:F:18:HIS:HE1	1:F:99:PHE:HE1	1.66	0.41
2:R:447:TYR:HB2	2:R:448:PRO:HD2	2.02	0.41
1:A:110:LYS:HG3	1:A:111:PRO:HD2	2.03	0.41
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.88	0.41
1:E:199:ASP:O	2:Q:338:SER:HA	2.21	0.41
1:F:77:GLY:O	1:F:114:VAL:HG12	2.21	0.41
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.46	0.41
2:N:315:TRP:HZ2	2:N:503:GLN:NE2	2.18	0.41
1:C:131:PHE:O	1:C:132:ALA:CB	2.67	0.41
2:O:497:ASN:HD21	2:O:499:GLU:HB2	1.86	0.41
2:P:410:HIS:CE1	2:P:412:ASN:H	2.33	0.41
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	2.02	0.41
2:R:488:MET:C	2:R:493:LYS:HE2	2.46	0.41
1:A:70:VAL:HG21	1:A:106:LEU:HD21	2.03	0.40
1:A:176:GLU:OE2	1:A:179:GLY:CA	2.68	0.40
1:B:115:ASN:HA	1:B:121:PRO:HA	2.03	0.40
1:B:140:HIS:O	1:B:197:PHE:HA	2.20	0.40
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.94	0.40
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.78	0.40
2:O:359:HIS:O	2:O:366:ASN:HB3	2.21	0.40
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.35	0.40
1:D:35:ILE:HD13	2:P:351:PHE:CE1	2.57	0.40
1:E:50:LEU:O	1:E:182:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:GLN:HG2	1:A:102:GLY:O	2.21	0.40
1:A:145:PHE:O	1:A:152:ASN:ND2	2.51	0.40
2:M:350:ASN:OD1	2:M:350:ASN:C	2.64	0.40
2:M:508:LEU:HD23	2:P:488:MET:HE1	2.02	0.40
1:B:15:PRO:HB3	1:B:133:ARG:HD2	2.03	0.40
2:O:350:ASN:OD1	2:O:350:ASN:C	2.64	0.40
1:D:18:HIS:CE1	1:D:99:PHE:CE1	3.09	0.40
1:E:100:ASP:CG	1:E:101:ALA:N	2.76	0.40
2:Q:483:ASP:HA	2:Q:484:PRO:HD2	1.80	0.40
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.84	0.40
2:M:361:HIS:CD2	2:M:361:HIS:N	2.68	0.40
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.66	0.40
2:M:336:LEU:O	2:O:325:LYS:NZ	2.53	0.40
2:O:410:HIS:ND1	2:O:412:ASN:N	2.56	0.40
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.22	0.40
1:F:114:VAL:HG23	1:F:122:MET:HE3	2.03	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%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	F	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
2	M	228/238 (96%)	219 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
2	O	228/238 (96%)	219 (96%)	9 (4%)	0	100	100
2	P	228/238 (96%)	221 (97%)	7 (3%)	0	100	100
2	Q	228/238 (96%)	222 (97%)	6 (3%)	0	100	100
2	R	228/238 (96%)	216 (95%)	12 (5%)	0	100	100
All	All	2556/2628 (97%)	2457 (96%)	99 (4%)	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%)	153 (94%)	9 (6%)	19	24
1	B	162/163 (99%)	154 (95%)	8 (5%)	22	29
1	C	162/163 (99%)	156 (96%)	6 (4%)	30	41
1	D	162/163 (99%)	155 (96%)	7 (4%)	26	35
1	E	162/163 (99%)	154 (95%)	8 (5%)	22	29
1	F	162/163 (99%)	155 (96%)	7 (4%)	26	35
2	M	195/201 (97%)	185 (95%)	10 (5%)	21	27
2	N	195/201 (97%)	184 (94%)	11 (6%)	19	24
2	O	195/201 (97%)	184 (94%)	11 (6%)	19	24
2	P	195/201 (97%)	186 (95%)	9 (5%)	24	32
2	Q	195/201 (97%)	186 (95%)	9 (5%)	24	32
2	R	195/201 (97%)	184 (94%)	11 (6%)	19	24
All	All	2142/2184 (98%)	2036 (95%)	106 (5%)	22	29

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	43	ASP
1	A	52	LEU
1	A	106	LEU
1	A	114	VAL
1	A	165	GLN
1	A	192	GLU
2	M	301	PRO
2	M	372	LEU
2	M	395	THR
2	M	411	LYS
2	M	416	LEU
2	M	433	SER
2	M	434	ASP
2	M	440	ARG
2	M	478	LEU
2	M	507	LYS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	52	LEU
1	B	106	LEU
1	B	158	LEU
1	B	165	GLN
1	B	176	GLU
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	411	LYS
2	N	416	LEU
2	N	428	ARG
2	N	433	SER
2	N	442	ILE
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	164	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	165	GLN
2	O	364	LEU
2	O	372	LEU
2	O	390	LYS
2	O	393	PRO
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	478	LEU
2	O	507	LYS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	114	VAL
1	D	165	GLN
1	D	180	LYS
2	P	372	LEU
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	497	ASN
1	E	4	LEU
1	E	19	ILE
1	E	32	ASP
1	E	38	ARG
1	E	49	ILE
1	E	52	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	306	SER
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	433	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Q	478	LEU
2	Q	499	GLU
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	23	LEU
1	F	52	LEU
1	F	94	ARG
1	F	165	GLN
1	F	181	THR
2	R	306	SER
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	478	LEU
2	R	497	ASN
2	R	503	GLN
2	R	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	28	ASN
1	A	80	GLN
1	A	127	ASN
1	A	136	ASN
1	A	150	GLN
1	A	163	GLN
1	A	165	GLN
2	M	305	ASN
2	M	361	HIS
2	M	497	ASN
2	M	503	GLN
1	B	11	GLN
1	B	165	GLN
2	N	359	HIS
2	N	361	HIS
2	N	412	ASN
2	N	422	ASN

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Mol	Chain	Res	Type
2	N	497	ASN
2	N	503	GLN
1	C	28	ASN
1	C	87	ASN
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	127	ASN
1	D	163	GLN
1	D	165	GLN
2	P	305	ASN
2	P	334	GLN
2	P	359	HIS
2	P	361	HIS
2	P	394	ASN
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	165	GLN
2	Q	359	HIS
2	Q	361	HIS
2	Q	497	ASN
2	Q	503	GLN
1	F	11	GLN
1	F	59	ASN
1	F	115	ASN
1	F	165	GLN
2	R	361	HIS
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
2	R	514	ASN
2	R	530	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CME	O	429	2	8,9,10	0.82	0	6,9,11	0.98	0
2	CME	P	429	2	8,9,10	0.79	0	6,9,11	1.59	1 (16%)
2	CME	N	429	2	8,9,10	0.52	0	6,9,11	0.58	0
2	CME	R	429	2	8,9,10	0.74	0	6,9,11	0.74	0
2	CME	Q	429	2	8,9,10	0.75	0	6,9,11	1.36	1 (16%)
2	CME	M	429	2	8,9,10	0.81	0	6,9,11	0.73	0

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	429	CME	CZ-CE-SD	-2.74	104.21	113.39
2	P	429	CME	CB-SG-SD	2.56	110.49	103.86

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 9 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	3HB	M	550	-	10,10,10	1.37	2 (20%)	13,13,13	1.19	1 (7%)
4	3HB	R	551	-	10,10,10	1.13	1 (10%)	13,13,13	1.03	2 (15%)
4	3HB	P	550	-	10,10,10	1.25	1 (10%)	13,13,13	1.19	2 (15%)
4	3HB	O	550	-	10,10,10	1.36	2 (20%)	13,13,13	1.48	2 (15%)
4	3HB	O	551	-	10,10,10	1.21	1 (10%)	13,13,13	1.05	1 (7%)
4	3HB	Q	550	-	10,10,10	1.50	2 (20%)	13,13,13	1.65	2 (15%)
4	3HB	N	551	-	10,10,10	1.24	1 (10%)	13,13,13	1.27	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	3HB	P	551	-	10,10,10	1.29	1 (10%)	13,13,13	1.12	2 (15%)
4	3HB	Q	551	-	10,10,10	1.24	1 (10%)	13,13,13	1.06	1 (7%)
4	3HB	M	551	-	10,10,10	1.23	1 (10%)	13,13,13	1.21	2 (15%)
4	3HB	N	550	-	10,10,10	1.34	2 (20%)	13,13,13	1.24	2 (15%)
4	3HB	R	550	-	10,10,10	1.38	2 (20%)	13,13,13	1.70	3 (23%)

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

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	551	3HB	C1-C1'	2.82	1.55	1.49
4	Q	550	3HB	C2-C1	2.82	1.43	1.39
4	Q	551	3HB	C1-C1'	2.68	1.55	1.49
4	P	551	3HB	C1-C1'	2.67	1.55	1.49
4	R	551	3HB	C1-C1'	2.55	1.54	1.49
4	M	551	3HB	C1-C1'	2.47	1.54	1.49
4	O	550	3HB	O2'-C1'	-2.38	1.23	1.30
4	O	551	3HB	C1-C1'	2.37	1.54	1.49
4	R	550	3HB	C5-C4	2.36	1.42	1.38
4	O	550	3HB	C2-C1	2.34	1.43	1.39
4	M	550	3HB	C5-C4	2.31	1.42	1.38
4	P	550	3HB	C2-C1	2.20	1.42	1.39
4	Q	550	3HB	C1-C1'	2.13	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	550	3HB	C2-C1	2.05	1.42	1.39
4	M	550	3HB	C1-C1'	2.04	1.53	1.49
4	N	550	3HB	O2'-C1'	-2.03	1.24	1.30
4	R	550	3HB	O2'-C1'	-2.02	1.24	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	550	3HB	O2'-C1'-C1	3.64	124.19	114.84
4	O	550	3HB	O2'-C1'-C1	3.48	123.77	114.84
4	N	551	3HB	O2'-C1'-O1'	-3.39	116.06	123.35
4	M	551	3HB	O2'-C1'-O1'	-3.06	116.78	123.35
4	P	550	3HB	O2'-C1'-C1	2.94	122.38	114.84
4	M	550	3HB	O2'-C1'-C1	2.90	122.27	114.84
4	Q	550	3HB	O2'-C1'-C1	2.84	122.13	114.84
4	Q	550	3HB	C5-C6-C1	-2.78	117.64	120.36
4	M	551	3HB	O2'-C1'-C1	2.74	121.87	114.84
4	O	550	3HB	O2'-C1'-O1'	-2.70	117.54	123.35
4	P	551	3HB	O2'-C1'-O1'	-2.67	117.60	123.35
4	R	550	3HB	O2'-C1'-O1'	-2.59	117.78	123.35
4	N	551	3HB	O2'-C1'-C1	2.56	121.40	114.84
4	R	551	3HB	O2'-C1'-C1	2.48	121.21	114.84
4	P	550	3HB	O2'-C1'-O1'	-2.43	118.13	123.35
4	R	550	3HB	C5-C6-C1	-2.35	118.06	120.36
4	Q	551	3HB	O2'-C1'-C1	2.26	120.65	114.84
4	N	550	3HB	O2'-C1'-C1	2.26	120.65	114.84
4	O	551	3HB	O2'-C1'-O1'	-2.25	118.51	123.35
4	N	550	3HB	O2'-C1'-O1'	-2.16	118.72	123.35
4	P	551	3HB	O2'-C1'-C1	2.08	120.17	114.84
4	R	551	3HB	O2'-C1'-O1'	-2.02	119.00	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	550	3HB	3	0
4	P	550	3HB	2	0
4	O	550	3HB	2	0
4	Q	550	3HB	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	550	3HB	1	0
4	R	550	3HB	3	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.