



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 PM UTC

PDB ID : 3PCG / pdb_00003pcg
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH THE INHIBITOR 4-HYDROXYPHENYLACETATE
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-04-29
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

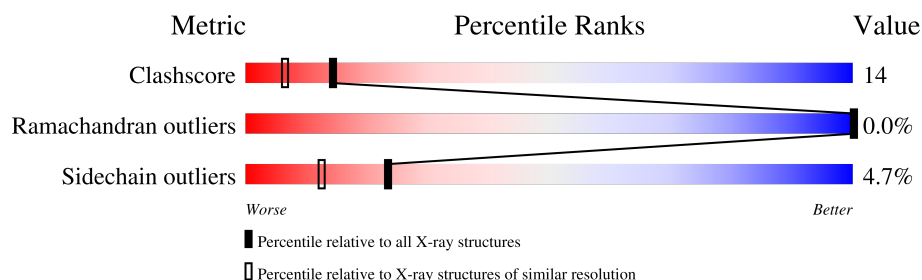
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	
2	M	238	
2	N	238	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	4HP	M	550	-	-	X	-
5	4HP	O	550	-	-	X	-
5	4HP	P	550	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

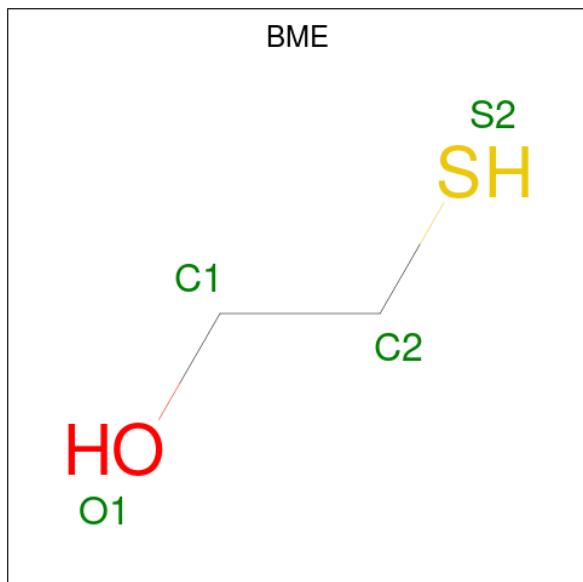
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

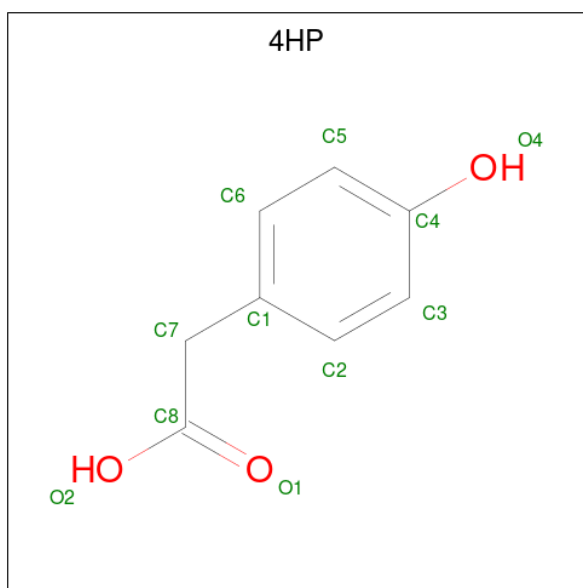
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

- Molecule 5 is 4-HYDROXYPHENYLACETATE (CCD ID: 4HP) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	0
			11	8	3		
5	N	1	Total	C	O	0	0
			11	8	3		
5	O	1	Total	C	O	0	0
			11	8	3		
5	P	1	Total	C	O	0	0
			11	8	3		
5	Q	1	Total	C	O	0	0
			11	8	3		
5	R	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	M	161	Total	O	0	0
			161	161		
6	B	84	Total	O	0	0
			84	84		
6	N	161	Total	O	0	0
			161	161		
6	C	81	Total	O	0	0
			81	81		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	O	157	Total 157	O 157	0	0
6	D	74	Total 74	O 74	0	0
6	P	158	Total 158	O 158	0	0
6	E	81	Total 81	O 81	0	0
6	Q	163	Total 163	O 163	0	0
6	F	78	Total 78	O 78	0	0
6	R	160	Total 160	O 160	0	0

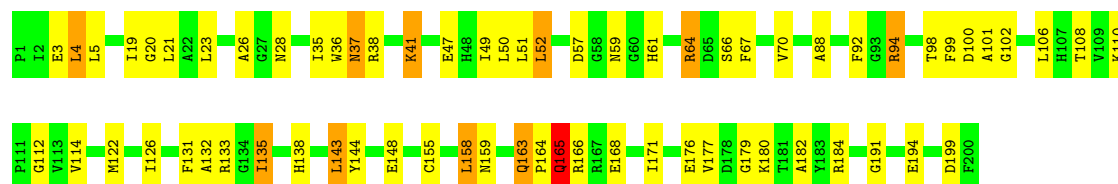
3 Residue-property plots [i](#)

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.

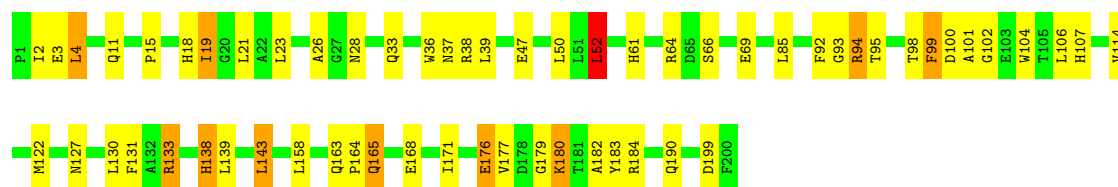
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



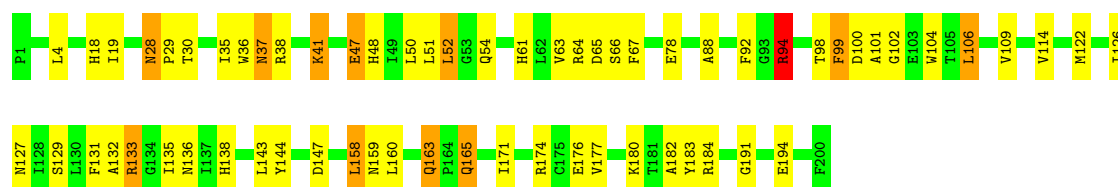
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



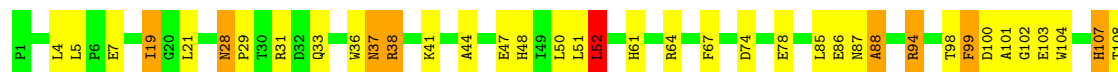
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 

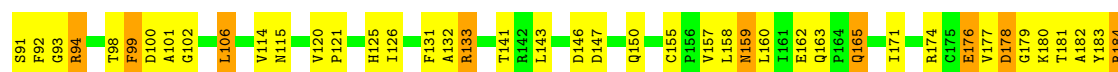
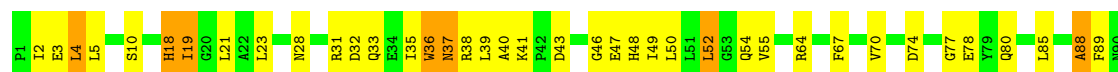




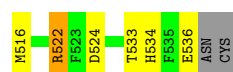
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



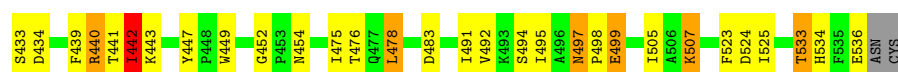
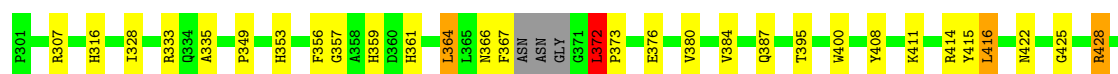
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



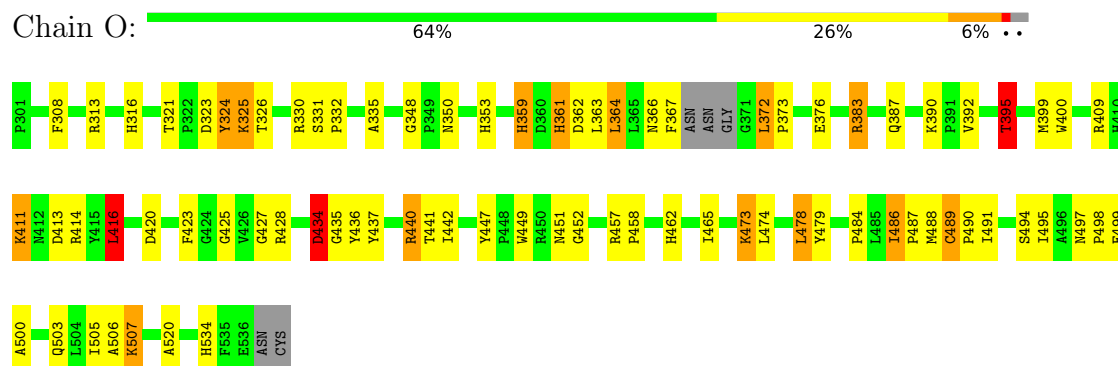
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



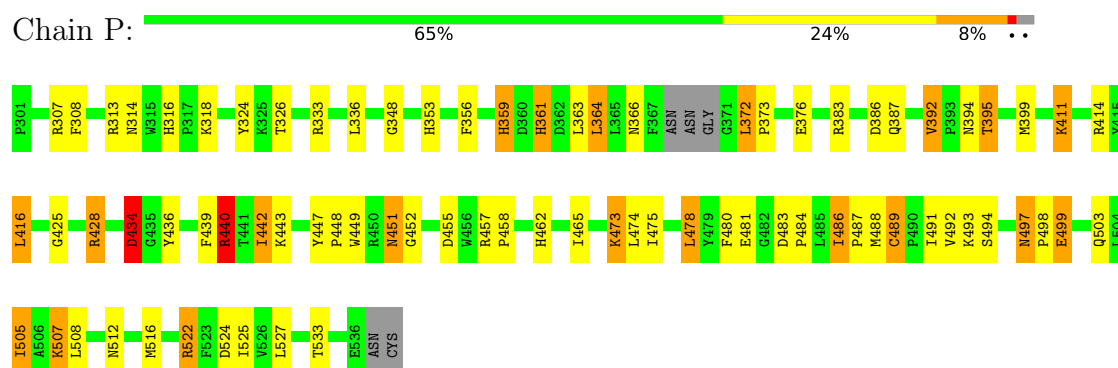
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



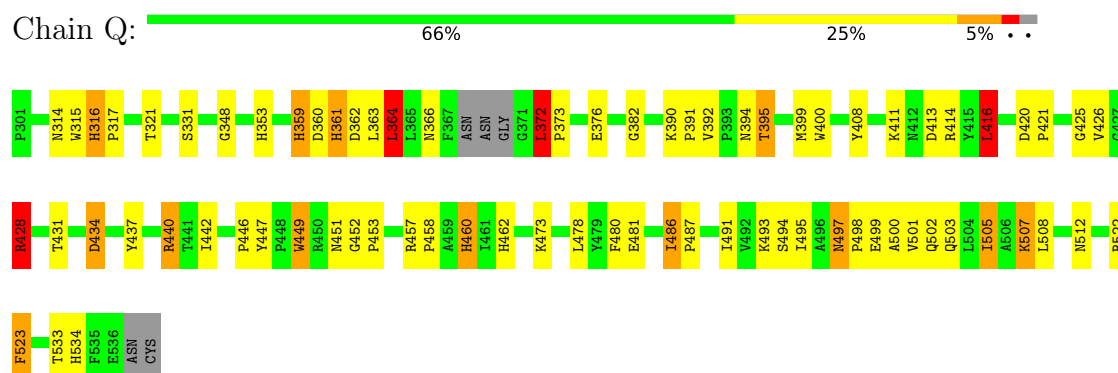
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



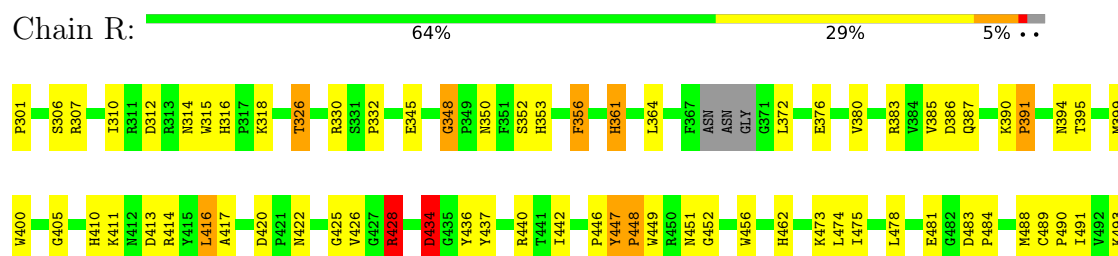
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.32Å 127.12Å 134.13Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 1.96	Depositor
% Data completeness (in resolution range)	81.4 (6.00-1.96)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21996	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 4HP, BME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	3/1611 (0.2%)	1.95	31/2195 (1.4%)
1	B	1.23	3/1611 (0.2%)	1.77	19/2195 (0.9%)
1	C	1.24	1/1611 (0.1%)	1.78	25/2195 (1.1%)
1	D	1.27	6/1611 (0.4%)	1.84	22/2195 (1.0%)
1	E	1.34	6/1611 (0.4%)	1.92	29/2195 (1.3%)
1	F	1.32	5/1611 (0.3%)	1.81	36/2195 (1.6%)
2	M	1.42	3/1895 (0.2%)	1.84	32/2580 (1.2%)
2	N	1.39	5/1895 (0.3%)	1.82	28/2580 (1.1%)
2	O	1.42	6/1895 (0.3%)	1.90	37/2580 (1.4%)
2	P	1.39	6/1895 (0.3%)	1.91	48/2580 (1.9%)
2	Q	1.45	7/1895 (0.4%)	1.87	38/2580 (1.5%)
2	R	1.40	4/1895 (0.2%)	1.89	33/2580 (1.3%)
All	All	1.35	55/21036 (0.3%)	1.86	378/28650 (1.3%)

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	94	ARG	CD-NE	-11.36	1.30	1.46
1	A	94	ARG	CD-NE	-10.57	1.31	1.46
2	O	451	ASN	CA-C	8.94	1.56	1.52
2	M	428	ARG	CD-NE	-8.00	1.35	1.46
2	Q	440	ARG	CD-NE	-7.87	1.35	1.46
1	A	47	GLU	CA-CB	-7.84	1.43	1.53
1	C	94	ARG	CD-NE	-7.56	1.35	1.46
2	P	428	ARG	CD-NE	-7.46	1.35	1.46
2	P	440	ARG	CD-NE	-7.43	1.35	1.46
2	R	428	ARG	CD-NE	-7.38	1.35	1.46
1	D	94	ARG	CD-NE	-7.26	1.36	1.46
1	D	108	THR	CA-CB	7.13	1.62	1.54
2	O	486	ILE	CA-CB	7.07	1.57	1.54
2	Q	451	ASN	CA-C	7.05	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	452	GLY	N-CA	6.68	1.51	1.43
1	E	47	GLU	CA-CB	-6.64	1.44	1.53
2	R	451	ASN	CA-C	6.61	1.55	1.52
2	N	440	ARG	CD-NE	-6.60	1.37	1.46
2	M	452	GLY	CA-C	6.49	1.60	1.51
1	D	133	ARG	CD-NE	-6.48	1.37	1.46
2	N	452	GLY	N-CA	5.95	1.52	1.44
2	O	506	ALA	N-CA	5.95	1.53	1.46
2	P	527	LEU	N-CA	5.79	1.52	1.45
2	Q	523	PHE	N-CA	5.75	1.53	1.46
1	A	108	THR	CA-CB	5.72	1.61	1.53
2	N	441	THR	CA-CB	5.69	1.61	1.53
1	B	138	HIS	CE1-NE2	5.68	1.38	1.32
1	B	2	ILE	CA-CB	5.65	1.61	1.54
2	O	441	THR	CA-CB	5.64	1.61	1.53
1	F	2	ILE	CA-CB	5.59	1.61	1.54
2	N	495	ILE	CA-CB	5.58	1.60	1.53
1	F	55	VAL	N-CA	5.42	1.52	1.46
1	D	133	ARG	NE-CZ	-5.40	1.27	1.33
1	E	108	THR	CA-CB	5.32	1.61	1.53
2	R	483	ASP	N-CA	5.31	1.54	1.46
2	Q	486	ILE	CA-CB	5.29	1.57	1.54
2	Q	321	THR	N-CA	5.28	1.52	1.46
1	F	74	ASP	N-CA	5.27	1.52	1.46
1	E	5	LEU	CA-C	5.25	1.59	1.53
1	F	5	LEU	CA-C	5.23	1.58	1.53
2	N	428	ARG	CD-NE	-5.20	1.39	1.46
1	E	196	VAL	CA-C	5.19	1.58	1.52
2	Q	508	LEU	N-CA	5.18	1.52	1.46
2	O	321	THR	CA-CB	5.16	1.60	1.53
2	Q	460	HIS	CE1-NE2	-5.16	1.27	1.32
2	M	318	LYS	N-CA	5.12	1.52	1.45
2	R	481	GLU	CA-CB	5.12	1.62	1.53
1	E	161	ILE	N-CA	5.12	1.52	1.46
1	F	10	SER	N-CA	5.11	1.52	1.45
1	D	123	ALA	N-CA	5.10	1.52	1.45
1	B	47	GLU	CA-CB	-5.08	1.46	1.53
1	D	127	ASN	N-CA	5.03	1.52	1.46
2	P	505	ILE	CA-CB	5.02	1.59	1.54
2	P	428	ARG	CG-CD	-5.01	1.37	1.52
2	O	313	ARG	NE-CZ	5.01	1.38	1.33

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	CA-CB-CG	29.43	172.96	114.10
1	A	94	ARG	CD-NE-CZ	27.15	162.41	124.40
1	D	133	ARG	CD-NE-CZ	25.55	160.17	124.40
1	E	47	GLU	CA-CB-CG	23.33	160.77	114.10
1	E	94	ARG	CD-NE-CZ	20.72	153.41	124.40
1	C	94	ARG	CD-NE-CZ	18.20	149.88	124.40
1	E	94	ARG	CG-CD-NE	13.22	141.09	112.00
2	R	428	ARG	CD-NE-CZ	13.13	142.79	124.40
1	F	47	GLU	CA-CB-CG	12.56	139.22	114.10
1	D	47	GLU	CA-CB-CG	12.32	138.74	114.10
1	B	47	GLU	CA-CB-CG	11.97	138.05	114.10
1	A	94	ARG	CG-CD-NE	11.63	137.60	112.00
2	N	440	ARG	NE-CZ-NH2	-11.21	109.11	119.20
2	M	440	ARG	NE-CZ-NH2	-11.21	109.12	119.20
2	P	440	ARG	NE-CZ-NH2	-11.14	109.17	119.20
1	D	94	ARG	CD-NE-CZ	11.03	139.84	124.40
2	P	428	ARG	CB-CG-CD	11.02	136.64	111.30
2	Q	440	ARG	NE-CZ-NH2	-10.98	109.31	119.20
2	P	428	ARG	CG-CD-NE	10.87	135.90	112.00
2	O	434	ASP	CA-CB-CG	-10.83	101.77	112.60
2	R	452	GLY	N-CA-C	-10.71	99.27	112.23
2	O	440	ARG	NE-CZ-NH2	-10.70	109.57	119.20
2	O	447	TYR	O-C-N	10.65	129.31	121.85
1	C	133	ARG	CD-NE-CZ	10.48	139.07	124.40
2	P	428	ARG	CD-NE-CZ	10.40	138.96	124.40
2	N	452	GLY	N-CA-C	-10.30	99.76	112.23
2	P	452	GLY	N-CA-C	-9.79	100.25	112.00
2	R	434	ASP	CA-CB-CG	-9.72	102.88	112.60
2	M	452	GLY	N-CA-C	-9.68	100.19	112.10
2	M	428	ARG	CG-CD-NE	9.57	133.06	112.00
2	M	428	ARG	CD-NE-CZ	9.57	137.79	124.40
2	R	361	HIS	CA-CB-CG	-9.57	104.23	113.80
1	C	99	PHE	CA-CB-CG	9.26	123.06	113.80
2	Q	394	ASN	CA-CB-CG	-9.19	103.41	112.60
2	R	440	ARG	NE-CZ-NH2	-9.18	110.94	119.20
2	O	452	GLY	N-CA-C	-9.18	101.13	112.23
2	O	387	GLN	OE1-CD-NE2	9.16	131.76	122.60
2	R	353	HIS	CA-CB-CG	-9.10	104.70	113.80
2	Q	512	ASN	CA-CB-CG	-8.95	103.65	112.60
2	P	434	ASP	CA-CB-CG	-8.93	103.67	112.60
1	D	94	ARG	NE-CZ-NH2	-8.90	111.19	119.20
2	P	361	HIS	CA-CB-CG	-8.90	104.90	113.80
2	P	372	LEU	CB-CA-C	8.82	120.94	108.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	447	TYR	O-C-N	8.76	128.66	121.83
1	E	94	ARG	NE-CZ-NH1	8.73	130.23	121.50
2	Q	359	HIS	CA-CB-CG	-8.72	105.08	113.80
2	Q	452	GLY	N-CA-C	-8.71	101.38	112.10
2	O	451	ASN	O-C-N	8.62	127.21	120.83
2	P	353	HIS	CA-CB-CG	-8.49	105.31	113.80
1	C	47	GLU	CA-CB-CG	8.31	130.72	114.10
1	C	133	ARG	NE-CZ-NH1	8.29	129.79	121.50
2	O	353	HIS	CA-CB-CG	-8.25	105.55	113.80
2	O	348	GLY	O-C-N	8.18	129.95	121.77
2	Q	361	HIS	CA-CB-CG	-8.18	105.62	113.80
2	O	325	LYS	N-CA-C	8.05	120.77	111.11
1	E	37	ASN	N-CA-C	7.97	122.38	113.21
2	Q	451	ASN	O-C-N	7.91	126.68	120.83
2	M	361	HIS	CA-CB-CG	-7.87	105.93	113.80
1	A	94	ARG	CB-CG-CD	7.81	129.26	111.30
2	R	428	ARG	CG-CD-NE	7.80	129.16	112.00
1	C	37	ASN	N-CA-C	7.71	122.27	113.02
2	Q	440	ARG	CD-NE-CZ	7.71	135.19	124.40
2	O	428	ARG	CD-NE-CZ	7.69	135.17	124.40
2	P	440	ARG	CD-NE-CZ	7.67	135.14	124.40
1	F	125	HIS	CA-CB-CG	-7.67	106.13	113.80
1	F	43	ASP	CA-CB-CG	-7.60	105.00	112.60
2	R	451	ASN	O-C-N	7.52	126.39	120.83
1	F	99	PHE	CA-CB-CG	7.45	121.25	113.80
2	P	457	ARG	CD-NE-CZ	7.37	134.72	124.40
1	C	94	ARG	NE-CZ-NH1	7.36	128.86	121.50
2	R	394	ASN	CA-CB-CG	-7.36	105.24	112.60
1	A	99	PHE	CA-CB-CG	7.31	121.11	113.80
1	B	37	ASN	N-CA-C	7.24	121.82	112.92
2	O	409	ARG	CD-NE-CZ	-7.20	114.32	124.40
1	D	94	ARG	NE-CZ-NH1	7.20	128.70	121.50
2	N	434	ASP	CA-CB-CG	-7.09	105.51	112.60
1	F	5	LEU	N-CA-C	-7.06	100.86	109.83
2	P	481	GLU	CB-CG-CD	7.05	124.59	112.60
2	M	494	SER	N-CA-C	-7.05	103.64	111.82
1	C	94	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	E	5	LEU	N-CA-C	-6.97	100.46	110.08
2	N	428	ARG	CB-CG-CD	6.97	127.32	111.30
1	A	3	GLU	CB-CG-CD	6.96	124.43	112.60
2	P	428	ARG	NE-CZ-NH2	-6.95	112.95	119.20
2	R	380	VAL	O-C-N	6.83	130.30	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	ASN	N-CA-C	6.83	121.21	113.02
2	R	326	THR	CA-CB-OG1	-6.83	99.36	109.60
2	R	422	ASN	CA-CB-CG	-6.79	105.81	112.60
2	N	428	ARG	CG-CD-NE	6.78	126.91	112.00
2	M	514	ASN	O-C-N	6.76	128.82	121.12
2	O	350	ASN	CA-CB-CG	-6.75	105.85	112.60
2	P	428	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	F	162	GLU	N-CA-CB	6.72	120.03	109.82
2	O	367	PHE	CA-C-O	-6.68	109.44	120.80
1	E	47	GLU	CB-CG-CD	6.64	123.89	112.60
2	P	394	ASN	CA-CB-CG	-6.62	105.97	112.60
2	O	451	ASN	CA-C-O	-6.62	116.00	119.77
1	E	94	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	F	37	ASN	N-CA-C	6.58	120.91	113.02
2	R	428	ARG	NE-CZ-NH2	-6.58	113.28	119.20
2	Q	457	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	B	177	VAL	CB-CA-C	6.54	119.26	110.42
2	M	439	PHE	O-C-N	6.54	130.86	123.27
1	B	11	GLN	CA-C-O	-6.51	113.70	120.99
1	A	5	LEU	N-CA-C	-6.50	101.39	109.64
1	E	133	ARG	N-CA-C	-6.47	100.85	110.23
2	R	314	ASN	N-CA-C	-6.47	105.54	113.50
1	D	132	ALA	O-C-N	6.46	129.33	123.26
1	F	21	LEU	N-CA-CB	-6.46	101.18	110.80
1	A	64	ARG	CD-NE-CZ	-6.45	115.37	124.40
1	F	133	ARG	N-CA-C	-6.45	101.15	110.24
2	Q	457	ARG	CD-NE-CZ	6.44	133.42	124.40
1	E	99	PHE	CA-CB-CG	6.41	120.20	113.80
2	Q	497	ASN	CB-CA-C	6.40	118.59	109.38
1	A	94	ARG	NE-CZ-NH2	-6.38	113.46	119.20
2	M	414	ARG	CD-NE-CZ	6.35	133.29	124.40
2	P	359	HIS	CA-CB-CG	-6.34	107.46	113.80
2	O	440	ARG	NH1-CZ-NH2	6.34	127.54	119.30
2	Q	372	LEU	CB-CA-C	6.34	118.30	108.61
2	N	367	PHE	CA-C-O	-6.33	110.05	120.80
1	F	3	GLU	CB-CG-CD	6.31	123.32	112.60
1	F	162	GLU	CA-CB-CG	6.28	126.67	114.10
2	P	486	ILE	O-C-N	6.27	124.43	120.42
2	P	326	THR	CA-CB-OG1	-6.26	100.20	109.60
2	O	395	THR	CA-CB-OG1	-6.24	100.24	109.60
1	D	94	ARG	CG-CD-NE	6.21	125.67	112.00
1	F	47	GLU	N-CA-CB	6.21	120.00	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	386	ASP	CA-CB-CG	6.21	118.81	112.60
2	R	356	PHE	CA-CB-CG	6.18	119.98	113.80
2	M	411	LYS	CB-CA-C	-6.18	100.49	110.74
2	N	380	VAL	O-C-N	6.17	129.74	123.20
1	B	28	ASN	O-C-N	6.17	126.59	121.35
1	D	28	ASN	O-C-N	6.16	127.54	121.57
1	A	166	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	F	36	TRP	CB-CA-C	6.11	122.58	110.42
2	R	411	LYS	CB-CA-C	-6.11	100.59	110.74
1	B	52	LEU	CB-CA-C	6.11	121.33	110.16
2	N	439	PHE	O-C-N	6.09	130.54	123.17
1	E	28	ASN	O-C-N	6.09	126.52	121.35
1	B	94	ARG	CD-NE-CZ	6.08	132.92	124.40
1	A	184	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	E	135	ILE	O-C-N	6.07	129.49	122.99
2	O	324	TYR	O-C-N	6.06	130.02	122.63
2	N	353	HIS	CA-CB-CG	-6.01	107.79	113.80
1	E	74	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	133	ARG	N-CA-C	-5.99	101.55	110.23
2	M	414	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	E	158	LEU	CB-CA-C	5.98	121.69	110.63
1	C	99	PHE	N-CA-C	-5.97	105.26	112.54
2	N	357	GLY	N-CA-C	-5.96	104.59	112.82
2	M	353	HIS	CA-CB-CG	-5.95	107.85	113.80
2	R	318	LYS	N-CA-C	-5.95	103.09	110.41
2	Q	501	VAL	O-C-N	5.94	127.64	121.87
1	F	184	ARG	CD-NE-CZ	-5.94	116.08	124.40
2	P	333	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	F	189	ILE	O-C-N	5.92	127.62	121.87
2	N	454	ASN	CA-CB-CG	5.92	118.52	112.60
2	N	440	ARG	NH1-CZ-NH2	5.91	126.98	119.30
2	Q	458	PRO	N-CA-C	-5.91	101.98	111.38
2	P	392	VAL	O-C-N	5.91	126.63	120.96
1	E	112	GLY	N-CA-C	-5.91	104.67	112.82
1	A	159	ASN	CA-CB-CG	-5.91	106.69	112.60
2	O	361	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	133	ARG	N-CA-C	-5.90	102.33	110.35
2	N	525	ILE	O-C-N	5.89	129.62	123.26
2	M	522	ARG	NE-CZ-NH2	5.87	124.48	119.20
2	M	428	ARG	CB-CG-CD	5.86	124.78	111.30
2	R	447	TYR	O-C-N	5.86	125.95	121.85
1	D	163	GLN	CA-C-O	5.84	123.64	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ASP	N-CA-C	-5.84	99.49	109.24
1	C	159	ASN	CA-CB-CG	-5.82	106.78	112.60
2	P	458	PRO	CB-CA-C	-5.80	103.35	110.95
2	P	383	ARG	NE-CZ-NH1	-5.80	115.70	121.50
2	Q	440	ARG	CB-CG-CD	-5.78	98.02	111.30
2	M	522	ARG	CD-NE-CZ	-5.77	116.32	124.40
2	Q	316	HIS	O-C-N	5.76	127.98	121.53
2	P	483	ASP	CA-C-O	5.76	125.15	119.51
2	O	494	SER	N-CA-C	-5.75	105.10	111.71
1	E	7	GLU	CB-CG-CD	5.75	122.37	112.60
2	P	439	PHE	O-C-N	5.74	130.30	123.24
2	O	316	HIS	O-C-N	5.73	128.20	121.66
2	M	417	ALA	N-CA-C	-5.73	102.55	109.83
1	C	133	ARG	N-CA-C	-5.73	102.56	110.35
1	D	59	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	C	30	THR	CA-CB-OG1	-5.72	101.02	109.60
1	B	36	TRP	CB-CA-C	5.71	121.78	110.42
1	D	159	ASN	CA-CB-CG	-5.70	106.90	112.60
2	M	489	CYS	N-CA-C	5.70	117.85	109.42
2	O	372	LEU	CB-CA-C	5.69	116.59	108.68
1	D	133	ARG	NE-CZ-NH1	5.68	127.18	121.50
2	R	316	HIS	O-C-N	5.67	127.61	121.60
2	N	372	LEU	N-CA-CB	-5.66	103.18	110.03
1	A	37	ASN	N-CA-C	5.65	119.80	113.02
1	F	158	LEU	CB-CA-C	5.65	120.17	110.79
1	F	99	PHE	N-CA-C	-5.65	105.65	112.54
2	M	314	ASN	CA-CB-CG	5.65	118.25	112.60
1	D	41	LYS	N-CA-C	-5.64	102.80	110.36
1	E	52	LEU	CB-CA-C	5.64	122.58	110.45
2	Q	533	THR	N-CA-C	-5.64	103.08	110.53
1	A	57	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	47	GLU	CB-CA-C	-5.63	101.36	110.77
2	M	336	LEU	CA-C-O	-5.62	115.44	121.56
1	E	37	ASN	CA-CB-CG	-5.61	106.99	112.60
2	P	314	ASN	N-CA-C	-5.60	106.61	113.50
1	A	158	LEU	CB-CA-C	5.59	120.08	110.79
1	A	26	ALA	N-CA-C	-5.59	106.30	113.01
1	F	150	GLN	O-C-N	5.59	127.84	122.03
2	O	420	ASP	CB-CA-C	5.58	116.37	110.17
2	N	316	HIS	CA-CB-CG	-5.58	108.22	113.80
1	F	141	THR	CA-CB-CG2	5.58	119.98	110.50
2	Q	434	ASP	CA-CB-CG	-5.57	107.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	359	HIS	CA-CB-CG	-5.57	108.23	113.80
2	Q	411	LYS	CB-CA-C	-5.56	101.50	110.74
1	A	177	VAL	CB-CA-C	5.54	117.33	110.73
1	A	66	SER	CB-CA-C	-5.54	98.73	109.76
2	P	316	HIS	CA-CB-CG	-5.54	108.26	113.80
2	M	314	ASN	N-CA-C	-5.53	106.53	113.28
2	Q	416	LEU	CB-CA-C	5.53	121.45	110.17
2	M	481	GLU	CB-CG-CD	5.53	121.99	112.60
1	C	158	LEU	CB-CA-C	5.52	119.96	110.79
2	P	314	ASN	CA-CB-CG	5.52	118.12	112.60
2	Q	428	ARG	NE-CZ-NH2	-5.51	114.24	119.20
2	Q	331	SER	O-C-N	5.51	126.29	121.39
2	R	428	ARG	NE-CZ-NH1	5.50	127.00	121.50
2	O	479	TYR	CA-C-O	-5.50	115.01	121.44
2	P	473	LYS	CA-CB-CG	5.50	125.09	114.10
2	Q	314	ASN	N-CA-C	-5.49	106.62	113.38
1	A	94	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	F	28	ASN	O-C-N	5.49	126.89	121.57
2	O	520	ALA	O-C-N	5.49	129.53	123.33
1	C	163	GLN	CA-C-O	5.49	123.68	119.46
2	Q	449	TRP	CA-C-O	-5.48	115.41	121.33
2	M	440	ARG	CB-CG-CD	-5.47	98.71	111.30
2	O	451	ASN	OD1-CG-ND2	5.47	128.07	122.60
2	N	483	ASP	O-C-N	5.46	126.06	121.31
1	B	183	TYR	N-CA-CB	5.45	120.89	111.13
1	F	171	ILE	N-CA-C	5.44	115.94	107.99
2	N	476	THR	O-C-N	5.44	128.81	122.99
2	P	507	LYS	CG-CD-CE	5.43	123.80	111.30
2	R	348	GLY	O-C-N	5.43	127.20	121.77
2	N	422	ASN	CA-CB-CG	-5.43	107.17	112.60
2	Q	382	GLY	O-C-N	5.43	129.86	123.62
2	R	440	ARG	CB-CG-CD	-5.43	98.82	111.30
2	R	526	VAL	O-C-N	5.43	128.80	122.99
2	Q	364	LEU	N-CA-C	-5.42	106.51	113.23
2	P	489	CYS	O-C-N	5.39	125.89	121.31
1	F	88	ALA	N-CA-C	-5.37	106.57	113.23
2	Q	512	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	F	94	ARG	CB-CG-CD	5.36	123.64	111.30
1	E	21	LEU	N-CA-CB	-5.36	102.81	110.80
2	P	383	ARG	CD-NE-CZ	-5.36	116.90	124.40
1	E	167	ARG	CD-NE-CZ	-5.36	116.90	124.40
1	B	99	PHE	CA-CB-CG	5.35	119.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	348	GLY	O-C-N	5.35	127.12	121.77
1	E	110	LYS	CB-CA-C	5.34	118.06	109.41
2	R	332	PRO	CB-CA-C	5.33	118.06	111.23
2	R	391	PRO	O-C-N	5.33	129.62	123.06
1	C	127	ASN	CA-CB-CG	-5.33	107.27	112.60
2	Q	372	LEU	N-CA-CB	-5.33	101.25	110.10
1	A	135	ILE	CA-CB-CG2	5.32	119.54	110.50
1	E	133	ARG	CD-NE-CZ	5.32	131.84	124.40
2	Q	446	PRO	N-CA-C	-5.31	103.73	111.33
1	E	141	THR	CA-CB-OG1	-5.31	101.63	109.60
1	D	166	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	D	21	LEU	N-CA-CB	-5.29	102.91	110.80
1	F	23	LEU	CB-CA-C	5.29	119.32	110.92
2	Q	534	HIS	CA-CB-CG	5.28	119.08	113.80
2	O	489	CYS	CA-C-N	5.28	125.08	119.28
2	O	489	CYS	C-N-CA	5.28	125.08	119.28
2	M	446	PRO	N-CA-C	-5.27	103.84	111.22
2	N	533	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	155	CYS	O-C-N	5.27	126.08	121.18
1	A	163	GLN	N-CA-C	5.27	118.17	108.69
2	P	522	ARG	NE-CZ-NH1	-5.27	116.23	121.50
2	Q	437	TYR	O-C-N	5.27	129.54	123.17
1	B	47	GLU	N-CA-CB	5.27	118.45	109.87
2	P	348	GLY	O-C-N	5.26	127.03	121.77
1	B	21	LEU	N-CA-CB	-5.26	102.97	110.80
2	Q	505	ILE	N-CA-C	5.25	115.66	107.99
1	F	32	ASP	CA-CB-CG	5.25	117.86	112.60
2	O	451	ASN	N-CA-C	-5.25	100.11	108.30
2	M	496	ALA	N-CA-C	5.25	117.08	111.36
2	M	465	ILE	O-C-N	5.24	128.86	123.20
1	C	171	ILE	CB-CA-C	5.24	118.16	110.98
2	R	446	PRO	N-CA-C	-5.24	103.89	111.22
1	A	23	LEU	CB-CA-C	5.22	119.23	110.92
2	M	325	LYS	N-CA-C	5.22	119.99	111.37
1	C	136	ASN	CA-CB-CG	-5.22	107.38	112.60
1	F	78	GLU	CB-CG-CD	5.22	121.48	112.60
1	C	106	LEU	N-CA-CB	-5.22	101.69	111.13
2	P	440	ARG	CB-CG-CD	-5.21	99.31	111.30
2	N	442	ILE	CB-CA-C	5.21	118.85	110.82
1	D	99	PHE	N-CA-C	-5.21	105.72	111.71
2	O	458	PRO	N-CA-C	-5.21	103.59	111.41
1	F	18	HIS	CA-CB-CG	-5.21	108.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	416	LEU	CB-CA-C	5.21	120.79	110.17
1	A	112	GLY	N-CA-C	-5.20	104.67	112.89
2	R	410	HIS	CA-C-N	5.20	128.62	120.82
2	R	410	HIS	C-N-CA	5.20	128.62	120.82
2	O	383	ARG	NE-CZ-NH2	-5.20	114.52	119.20
2	R	532	LYS	N-CA-C	-5.20	103.54	110.55
2	O	383	ARG	N-CA-CB	-5.19	102.20	111.08
1	F	46	GLY	CA-C-O	-5.19	118.71	122.45
2	O	308	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	155	CYS	O-C-N	5.19	126.00	121.18
2	Q	353	HIS	CA-CB-CG	-5.18	108.62	113.80
1	C	78	GLU	CB-CG-CD	5.18	121.40	112.60
1	B	127	ASN	CA-CB-CG	-5.18	107.42	112.60
1	F	178	ASP	N-CA-C	-5.17	104.99	111.92
2	R	448	PRO	CB-CA-C	5.17	117.74	110.60
2	N	440	ARG	CB-CG-CD	-5.16	99.42	111.30
1	F	159	ASN	CA-CB-CG	-5.16	107.44	112.60
2	P	499	GLU	CA-CB-CG	5.16	124.41	114.10
1	F	126	ILE	O-C-N	5.15	128.82	123.26
1	A	41	LYS	N-CA-C	-5.14	103.19	110.29
2	N	494	SER	N-CA-C	-5.14	106.27	112.54
2	P	494	SER	N-CA-C	-5.14	106.27	112.54
1	D	23	LEU	CB-CA-C	5.13	119.35	110.84
2	M	503	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	C	28	ASN	O-C-N	5.12	125.70	121.35
2	O	323	ASP	CA-CB-CG	-5.12	107.48	112.60
2	N	411	LYS	CB-CA-C	-5.12	102.24	110.74
2	O	457	ARG	N-CA-C	-5.12	103.33	109.83
2	Q	502	GLN	O-C-N	5.12	128.21	122.22
1	D	94	ARG	CB-CG-CD	5.12	123.07	111.30
1	F	106	LEU	N-CA-CB	-5.12	102.01	111.53
1	A	133	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	C	41	LYS	N-CA-C	-5.11	102.78	110.24
1	F	183	TYR	CA-CB-CG	5.11	123.09	113.90
2	R	420	ASP	CB-CA-C	5.11	116.02	110.15
1	A	59	ASN	CA-CB-CG	5.10	117.70	112.60
2	P	492	VAL	N-CA-C	-5.10	105.52	110.42
1	E	107	HIS	CA-CB-CG	-5.10	108.70	113.80
1	E	88	ALA	N-CA-C	-5.10	105.80	112.23
1	E	138	HIS	CA-CB-CG	-5.10	108.70	113.80
1	F	176	GLU	CB-CG-CD	5.10	121.27	112.60
2	M	326	THR	CA-CB-OG1	-5.10	101.96	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	499	GLU	N-CA-CB	5.09	118.18	110.28
2	N	447	TYR	CB-CA-C	5.09	116.84	109.92
1	A	99	PHE	N-CA-C	-5.09	106.33	112.54
1	B	184	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	P	497	ASN	CA-C-N	5.08	124.87	119.28
2	P	497	ASN	C-N-CA	5.08	124.87	119.28
1	F	47	GLU	CB-CA-C	-5.08	101.95	110.29
2	P	451	ASN	O-C-N	5.08	129.35	122.59
2	Q	522	ARG	NE-CZ-NH1	-5.08	116.42	121.50
2	P	308	PHE	CA-CB-CG	-5.07	108.73	113.80
1	D	4	LEU	N-CA-CB	-5.07	102.34	110.51
2	P	522	ARG	CD-NE-CZ	-5.06	117.31	124.40
2	P	512	ASN	CA-CB-CG	-5.06	107.54	112.60
2	P	451	ASN	N-CA-C	-5.05	100.03	110.80
2	N	524	ASP	O-C-N	5.05	128.72	123.06
1	A	165	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	107	HIS	CA-CB-CG	-5.05	108.75	113.80
2	Q	431	THR	N-CA-CB	5.04	117.44	110.17
1	B	139	LEU	O-C-N	5.04	129.09	123.19
1	D	47	GLU	N-CA-CB	5.04	118.64	110.17
2	P	314	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	E	148	GLU	CA-CB-CG	5.04	124.18	114.10
2	Q	494	SER	N-CA-C	-5.04	106.40	112.54
2	O	387	GLN	CB-CG-CD	-5.03	104.04	112.60
1	E	113	VAL	N-CA-CB	-5.03	103.36	110.26
1	F	125	HIS	CA-C-O	5.03	126.77	121.33
1	C	183	TYR	N-CA-CB	5.03	119.26	110.81
1	C	47	GLU	CA-C-O	-5.02	114.93	120.60
1	B	95	THR	CA-CB-OG1	-5.02	102.07	109.60
1	C	129	SER	N-CA-CB	5.02	119.11	110.68
2	M	380	VAL	N-CA-C	-5.02	100.52	107.80
2	R	307	ARG	N-CA-C	-5.02	101.57	109.50
2	N	492	VAL	N-CA-C	-5.01	105.61	110.42
1	A	64	ARG	NE-CZ-NH1	-5.01	116.49	121.50
2	N	384	VAL	CA-C-O	-5.01	115.13	120.59
2	P	336	LEU	CA-C-O	-5.01	116.10	121.56
2	M	384	VAL	O-C-N	5.01	128.96	123.10
2	M	440	ARG	NH1-CZ-NH2	5.01	125.81	119.30
2	P	505	ILE	N-CA-C	5.00	115.89	108.23
2	N	443	LYS	CG-CD-CE	5.00	122.80	111.30
1	E	47	GLU	N-CA-CB	5.00	118.02	109.87

There are no chirality outliers.

There are no planarity outliers.

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	48	0
1	B	1571	0	1499	49	0
1	C	1571	0	1499	50	0
1	D	1571	0	1499	42	0
1	E	1571	0	1499	49	0
1	F	1571	0	1499	69	0
2	M	1840	0	1792	59	0
2	N	1840	0	1792	35	0
2	O	1840	0	1792	51	0
2	P	1840	0	1792	56	0
2	Q	1840	0	1792	47	0
2	R	1840	0	1792	58	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	3	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	1	0
4	R	4	0	5	0	0
5	M	11	0	6	4	0
5	N	11	0	6	2	0
5	O	11	0	6	4	0
5	P	11	0	6	5	0
5	Q	11	0	6	2	0
5	R	11	0	6	3	0
6	A	76	0	0	2	0
6	B	84	0	0	1	0
6	C	81	0	0	1	0
6	D	74	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	81	0	0	1	0
6	F	78	0	0	3	0
6	M	161	0	0	2	0
6	N	161	0	0	1	0
6	O	157	0	0	2	0
6	P	158	0	0	1	0
6	Q	163	0	0	3	0
6	R	160	0	0	5	0
All	All	21996	0	19812	571	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 14.

All (571) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLN:H	1:D:165:GLN:NE2	1.29	1.30
1:D:165:GLN:HE21	1:D:165:GLN:N	1.42	1.15
1:E:165:GLN:H	1:E:165:GLN:NE2	1.45	1.12
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.05	1.10
1:E:165:GLN:HE21	1:E:165:GLN:N	1.49	1.09
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.68	1.08
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.35	1.07
1:A:98:THR:HB	1:A:100:ASP:OD1	1.58	1.04
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.19	1.03
1:C:64:ARG:NH1	1:C:100:ASP:O	1.93	1.01
1:B:165:GLN:H	1:B:165:GLN:NE2	1.60	1.00
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.77	1.00
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.46	0.97
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.18	0.95
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.82	0.95
1:F:165:GLN:NE2	1:F:165:GLN:H	1.67	0.91
1:F:98:THR:HB	1:F:100:ASP:OD1	1.70	0.91
1:C:165:GLN:H	1:C:165:GLN:NE2	1.67	0.91
1:B:18:HIS:ND1	6:B:473:HOH:O	2.02	0.91
1:C:98:THR:OG1	1:C:102:GLY:N	2.05	0.90
1:D:64:ARG:NH1	1:D:100:ASP:O	2.04	0.89
1:F:98:THR:OG1	1:F:102:GLY:N	2.06	0.88
2:R:361:HIS:H	2:R:361:HIS:CD2	1.88	0.88
1:D:98:THR:OG1	1:D:102:GLY:N	2.05	0.88
2:M:390:LYS:HD2	6:M:644:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:NE2	1:B:165:GLN:N	2.23	0.87
2:P:313:ARG:O	2:P:318:LYS:HE2	1.74	0.86
1:B:165:GLN:H	1:B:165:GLN:CD	1.76	0.86
1:B:176:GLU:HG3	1:B:180:LYS:O	1.76	0.85
1:F:180:LYS:HD2	1:F:181:THR:N	1.90	0.85
2:R:361:HIS:H	2:R:361:HIS:HD2	1.24	0.85
1:F:64:ARG:NH1	1:F:100:ASP:O	2.09	0.85
2:P:491:ILE:HD11	5:P:550:4HP:H71	1.57	0.84
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.59	0.84
2:O:497:ASN:HD22	2:O:499:GLU:H	1.25	0.84
1:F:165:GLN:H	1:F:165:GLN:CD	1.82	0.84
1:E:98:THR:OG1	1:E:102:GLY:N	2.11	0.83
1:C:165:GLN:H	1:C:165:GLN:HE21	1.23	0.83
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.07	0.83
1:D:98:THR:HB	1:D:100:ASP:OD1	1.77	0.83
1:A:98:THR:OG1	1:A:102:GLY:N	2.10	0.83
2:O:390:LYS:HE2	6:O:729:HOH:O	1.77	0.83
2:O:497:ASN:ND2	2:O:499:GLU:H	1.76	0.82
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.80	0.81
1:F:163:GLN:CB	1:F:165:GLN:HE22	1.92	0.81
1:B:163:GLN:CB	1:B:165:GLN:HE22	1.89	0.81
1:C:18:HIS:ND1	6:C:281:HOH:O	2.08	0.81
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.46	0.81
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.63	0.81
2:M:497:ASN:HD22	2:M:499:GLU:H	1.29	0.81
2:P:411:LYS:O	2:P:414:ARG:NH1	2.14	0.80
1:E:98:THR:HB	1:E:100:ASP:OD1	1.82	0.80
2:N:497:ASN:HD22	2:N:499:GLU:H	1.31	0.79
2:M:361:HIS:H	2:M:361:HIS:CD2	1.98	0.79
1:A:163:GLN:CB	1:A:165:GLN:HE22	1.96	0.78
2:Q:390:LYS:HD2	6:Q:1032:HOH:O	1.82	0.78
2:R:497:ASN:HD22	2:R:499:GLU:H	1.29	0.78
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	1.84	0.77
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.84	0.77
2:M:497:ASN:ND2	2:M:499:GLU:H	1.80	0.77
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.67	0.77
1:F:18:HIS:ND1	6:F:1429:HOH:O	2.17	0.76
1:A:165:GLN:CD	1:A:165:GLN:H	1.91	0.76
1:D:18:HIS:ND1	6:D:951:HOH:O	2.19	0.76
1:B:176:GLU:HG3	1:B:180:LYS:C	2.10	0.75
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ARG:NH1	1:E:100:ASP:O	2.20	0.75
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.01	0.75
2:R:497:ASN:ND2	2:R:499:GLU:H	1.85	0.75
2:M:491:ILE:HD11	5:M:550:4HP:H71	1.68	0.74
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.52	0.73
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.23	0.73
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.70	0.72
2:P:478:LEU:C	2:P:478:LEU:HD23	2.14	0.72
1:D:165:GLN:NE2	1:D:165:GLN:N	2.14	0.72
2:N:497:ASN:ND2	2:N:499:GLU:H	1.88	0.72
1:D:177:VAL:O	1:D:180:LYS:HB3	1.90	0.72
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.70	0.72
1:B:98:THR:HB	1:B:100:ASP:OD1	1.91	0.71
2:R:473:LYS:HD2	2:R:474:LEU:N	2.05	0.71
2:R:484:PRO:O	2:R:488:MET:HE3	1.90	0.71
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.39	0.71
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.73	0.71
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.26	0.71
2:O:491:ILE:HD11	5:O:550:4HP:H71	1.74	0.70
2:R:361:HIS:CD2	2:R:361:HIS:N	2.60	0.70
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.57	0.69
1:E:100:ASP:CG	1:E:101:ALA:H	1.99	0.69
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.18	0.69
1:C:98:THR:HB	1:C:100:ASP:OD1	1.91	0.69
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.74	0.69
2:M:361:HIS:H	2:M:361:HIS:HD2	1.37	0.69
1:D:165:GLN:H	1:D:165:GLN:HE21	0.72	0.69
1:F:64:ARG:HD3	1:F:99:PHE:O	1.92	0.68
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.75	0.68
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.11	0.68
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.08	0.68
2:R:390:LYS:HD3	6:R:1271:HOH:O	1.94	0.68
2:M:449:TRP:CE3	5:M:550:4HP:H72	2.28	0.67
2:P:324:TYR:OH	5:P:550:4HP:O1	2.10	0.67
1:A:64:ARG:NH1	1:A:100:ASP:O	2.27	0.67
2:Q:390:LYS:HD3	6:Q:1150:HOH:O	1.95	0.66
1:F:48:HIS:C	1:F:180:LYS:HZ2	2.02	0.66
1:F:180:LYS:HD2	1:F:181:THR:H	1.60	0.66
1:F:48:HIS:C	1:F:180:LYS:NZ	2.53	0.66
1:F:100:ASP:CG	1:F:101:ALA:H	2.03	0.66
1:C:165:GLN:HE21	1:C:165:GLN:N	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.94	0.65
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.77	0.65
1:F:77:GLY:O	1:F:114:VAL:HG12	1.97	0.65
2:N:491:ILE:HD11	5:N:550:4HP:H71	1.79	0.65
2:O:361:HIS:H	2:O:361:HIS:CD2	2.15	0.65
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.12	0.65
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.97	0.65
1:A:176:GLU:HG3	1:A:180:LYS:O	1.97	0.64
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.23	0.64
2:O:449:TRP:CE3	5:O:550:4HP:H72	2.31	0.64
1:A:100:ASP:CG	1:A:101:ALA:H	2.04	0.64
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.80	0.64
2:N:478:LEU:C	2:N:478:LEU:HD23	2.22	0.64
2:R:536:GLU:HB2	6:R:1352:HOH:O	1.98	0.64
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.62	0.63
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.79	0.63
1:D:165:GLN:H	1:D:165:GLN:CD	2.04	0.63
2:P:491:ILE:CD1	5:P:550:4HP:H71	2.27	0.63
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.30	0.63
1:C:100:ASP:OD1	1:C:100:ASP:N	2.30	0.63
1:B:3:GLU:HA	1:B:3:GLU:OE1	1.99	0.63
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.81	0.63
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.63	0.63
2:P:361:HIS:H	2:P:361:HIS:CD2	2.16	0.62
1:F:165:GLN:NE2	1:F:165:GLN:N	2.44	0.62
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.35	0.62
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.15	0.62
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.33	0.62
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.80	0.62
2:R:497:ASN:HD22	2:R:497:ASN:C	2.08	0.62
2:R:390:LYS:HE2	6:R:1389:HOH:O	1.99	0.62
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.81	0.62
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.97	0.61
1:F:98:THR:O	1:F:102:GLY:HA2	1.99	0.61
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.67	0.61
2:M:478:LEU:HD23	2:M:478:LEU:C	2.26	0.61
2:N:416:LEU:HD23	2:N:416:LEU:C	2.25	0.61
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.46	0.61
2:P:484:PRO:O	2:P:488:MET:HE3	2.00	0.61
1:F:155:CYS:O	1:F:159:ASN:ND2	2.34	0.61
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.83	0.61
2:O:399:MET:HA	2:O:462:HIS:O	2.00	0.60
2:M:413:ASP:C	2:M:414:ARG:HD2	2.26	0.60
1:B:64:ARG:NH1	1:B:100:ASP:O	2.33	0.60
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.82	0.60
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.37	0.60
2:O:497:ASN:HD22	2:O:497:ASN:C	2.10	0.60
1:D:176:GLU:HA	1:D:180:LYS:O	2.01	0.60
2:M:497:ASN:HD22	2:M:497:ASN:C	2.10	0.60
2:R:491:ILE:HD11	5:R:550:4HP:H71	1.84	0.60
1:B:176:GLU:HA	1:B:180:LYS:O	2.01	0.60
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.08	0.60
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.27	0.59
1:F:115:ASN:HA	1:F:121:PRO:HA	1.83	0.59
2:N:449:TRP:CE3	5:N:550:4HP:H72	2.36	0.59
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.17	0.59
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.84	0.59
1:B:52:LEU:HA	1:B:104:TRP:O	2.03	0.59
1:B:165:GLN:N	1:B:165:GLN:CD	2.55	0.59
1:D:180:LYS:HG3	1:D:181:THR:N	2.17	0.59
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.37	0.58
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.03	0.58
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.67	0.58
1:B:165:GLN:N	1:B:165:GLN:HE21	2.01	0.58
2:Q:449:TRP:CE3	5:Q:550:4HP:H72	2.37	0.58
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.49	0.58
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.84	0.58
1:D:64:ARG:HD3	1:D:99:PHE:O	2.04	0.58
1:E:61:HIS:CE1	1:F:163:GLN:HG3	2.38	0.58
1:C:99:PHE:HE2	2:O:411:LYS:HD2	1.68	0.58
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.39	0.58
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.67	0.57
1:C:177:VAL:O	1:C:180:LYS:HB3	2.04	0.57
2:R:400:TRP:HA	2:R:425:GLY:O	2.03	0.57
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.19	0.57
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.86	0.57
1:B:92:PHE:CG	2:N:349:PRO:HG3	2.40	0.57
1:D:100:ASP:CG	1:D:101:ALA:H	2.13	0.56
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.87	0.56
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.40	0.56
1:F:50:LEU:O	1:F:182:ALA:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:VAL:HG11	1:F:106:LEU:HD21	1.87	0.56
1:C:48:HIS:HA	1:C:109:VAL:HG12	1.87	0.56
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.36	0.56
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.88	0.56
1:D:52:LEU:C	1:D:52:LEU:HD22	2.30	0.56
2:O:478:LEU:HD23	2:O:478:LEU:C	2.31	0.56
1:C:36:TRP:CG	1:C:37:ASN:H	2.24	0.56
2:P:364:LEU:HD12	2:P:373:PRO:HG2	1.88	0.55
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.35	0.55
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.89	0.55
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.88	0.55
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.06	0.55
1:F:49:ILE:HA	1:F:180:LYS:HE3	1.89	0.55
2:P:462:HIS:HE1	5:P:550:4HP:H3	1.71	0.55
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.87	0.55
1:F:165:GLN:CD	1:F:165:GLN:N	2.60	0.55
2:O:361:HIS:CG	4:O:601:BME:H21	2.41	0.55
2:N:414:ARG:NE	2:N:414:ARG:HA	2.22	0.55
1:F:131:PHE:O	1:F:132:ALA:HB2	2.07	0.55
1:B:165:GLN:HE21	1:B:165:GLN:CA	2.18	0.55
2:O:324:TYR:OH	5:O:550:4HP:O1	2.22	0.54
2:R:473:LYS:HD2	2:R:474:LEU:H	1.72	0.54
2:M:416:LEU:C	2:M:416:LEU:HD23	2.32	0.54
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.37	0.54
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.42	0.54
2:P:473:LYS:HD2	2:P:474:LEU:N	2.21	0.54
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.72	0.54
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.42	0.54
1:B:143:LEU:C	1:B:143:LEU:HD23	2.33	0.54
1:F:54:GLN:HG3	1:F:184:ARG:NH2	2.23	0.54
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.89	0.54
2:O:434:ASP:HB3	2:O:436:TYR:CE2	2.42	0.54
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.23	0.54
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.73	0.53
2:N:359:HIS:O	2:N:366:ASN:HB3	2.08	0.53
2:N:497:ASN:HD22	2:N:499:GLU:N	2.03	0.53
1:E:168:GLU:HA	1:E:171:ILE:CD1	2.36	0.53
2:O:465:ILE:HD12	2:O:465:ILE:N	2.23	0.53
2:M:414:ARG:HD2	2:M:414:ARG:N	2.23	0.53
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.88	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.54	0.53
2:R:488:MET:C	2:R:493:LYS:HZ1	2.16	0.53
2:R:416:LEU:C	2:R:416:LEU:HD23	2.34	0.53
2:M:497:ASN:HD22	2:M:498:PRO:N	2.07	0.53
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.33	0.53
1:A:20:GLY:O	1:A:21:LEU:HD23	2.08	0.53
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.44	0.53
1:C:147:ASP:OD2	1:C:174:ARG:NH1	2.41	0.53
1:A:176:GLU:HA	1:A:180:LYS:O	2.08	0.53
1:F:35:ILE:HG21	1:F:92:PHE:CE2	2.43	0.53
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.44	0.53
2:P:361:HIS:H	2:P:361:HIS:HD2	1.56	0.53
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.52
1:D:98:THR:O	1:D:102:GLY:HA2	2.09	0.52
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.24	0.52
1:E:31:ARG:HH11	2:Q:428:ARG:HG2	1.75	0.52
2:P:497:ASN:C	2:P:497:ASN:HD22	2.17	0.52
2:P:497:ASN:ND2	2:P:499:GLU:H	2.07	0.52
1:F:180:LYS:HE3	1:F:181:THR:O	2.08	0.52
1:E:143:LEU:HD23	1:E:143:LEU:C	2.34	0.52
1:F:52:LEU:C	1:F:52:LEU:HD22	2.32	0.52
2:M:505:ILE:O	2:M:507:LYS:HE3	2.08	0.52
2:M:536:GLU:HB2	6:M:699:HOH:O	2.10	0.52
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.45	0.52
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.10	0.52
2:R:356:PHE:HD2	2:R:428:ARG:HD3	1.74	0.52
2:R:434:ASP:HB3	2:R:436:TYR:CE2	2.45	0.51
1:A:143:LEU:C	1:A:143:LEU:HD23	2.35	0.51
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.91	0.51
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.10	0.51
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.93	0.51
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.26	0.51
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.46	0.51
1:D:18:HIS:HD1	1:D:99:PHE:HZ	1.59	0.51
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.45	0.51
1:E:176:GLU:HG3	1:E:180:LYS:O	2.10	0.51
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	1.93	0.51
1:B:176:GLU:OE2	1:B:179:GLY:C	2.54	0.51
1:E:98:THR:O	1:E:102:GLY:HA2	2.10	0.51
1:F:19:ILE:O	2:R:426:VAL:HG21	2.11	0.51
1:F:100:ASP:OD1	1:F:100:ASP:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TRP:CG	1:D:37:ASN:H	2.27	0.51
1:A:98:THR:O	1:A:102:GLY:HA2	2.11	0.51
1:D:143:LEU:C	1:D:143:LEU:HD23	2.36	0.51
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.93	0.51
1:A:50:LEU:O	1:A:182:ALA:HA	2.10	0.51
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.41	0.51
2:M:362:ASP:CG	2:M:440:ARG:HD2	2.35	0.51
2:Q:473:LYS:NZ	6:Q:1135:HOH:O	2.43	0.51
2:M:448:PRO:HB2	2:P:516:MET:HA	1.93	0.50
1:C:98:THR:O	1:C:102:GLY:HA2	2.12	0.50
1:E:98:THR:OG1	1:E:101:ALA:HB3	2.11	0.50
2:R:383:ARG:NH2	2:R:434:ASP:OD1	2.43	0.50
1:B:176:GLU:HG3	1:B:180:LYS:N	2.26	0.50
2:O:497:ASN:HD21	2:O:499:GLU:HB2	1.75	0.50
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.94	0.50
2:R:413:ASP:C	2:R:414:ARG:HD2	2.36	0.50
1:D:38:ARG:HG3	1:D:107:HIS:HB2	1.92	0.50
1:B:64:ARG:HD3	1:B:99:PHE:O	2.12	0.50
2:N:376:GLU:O	2:N:442:ILE:HA	2.11	0.50
2:O:416:LEU:C	2:O:416:LEU:HD23	2.36	0.50
2:O:484:PRO:O	2:O:487:PRO:HD2	2.12	0.50
2:R:497:ASN:HD22	2:R:499:GLU:N	2.04	0.50
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.27	0.50
1:F:18:HIS:CG	6:F:1429:HOH:O	2.59	0.50
1:D:18:HIS:CG	6:D:951:HOH:O	2.64	0.50
2:P:356:PHE:HD2	2:P:428:ARG:HD3	1.77	0.49
2:P:497:ASN:HD22	2:P:499:GLU:H	1.60	0.49
2:O:376:GLU:O	2:O:442:ILE:HA	2.11	0.49
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.94	0.49
2:M:491:ILE:CD1	5:M:550:4HP:H71	2.41	0.49
2:M:361:HIS:ND1	4:M:601:BME:H21	2.28	0.49
2:O:497:ASN:HD22	2:O:499:GLU:N	2.02	0.49
2:Q:491:ILE:HD11	5:Q:550:4HP:H71	1.95	0.49
2:M:522:ARG:HE	2:M:524:ASP:CG	2.21	0.49
1:C:52:LEU:C	1:C:52:LEU:HD22	2.38	0.49
2:P:364:LEU:CD1	2:P:442:ILE:HG23	2.43	0.49
2:O:473:LYS:HD2	2:O:474:LEU:N	2.28	0.49
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.94	0.48
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.77	0.48
1:E:41:LYS:HD2	1:E:87:ASN:O	2.12	0.48
1:F:36:TRP:CG	1:F:37:ASN:H	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:491:ILE:CD1	5:O:550:4HP:H71	2.43	0.48
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.39	0.48
2:R:385:VAL:O	2:R:526:VAL:HA	2.12	0.48
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.94	0.48
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.13	0.48
1:B:114:VAL:HG23	1:B:122:MET:HE3	1.94	0.48
2:N:361:HIS:CD2	2:N:361:HIS:H	2.30	0.48
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.49	0.48
2:O:497:ASN:HD22	2:O:498:PRO:N	2.12	0.48
1:E:176:GLU:HA	1:E:180:LYS:O	2.12	0.48
1:C:50:LEU:O	1:C:182:ALA:HA	2.13	0.48
2:P:416:LEU:C	2:P:416:LEU:HD23	2.38	0.48
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.29	0.48
1:E:36:TRP:CG	1:E:37:ASN:H	2.32	0.48
1:F:143:LEU:C	1:F:143:LEU:HD23	2.38	0.48
1:A:28:ASN:HB3	6:A:262:HOH:O	2.13	0.48
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.77	0.48
2:R:449:TRP:CE3	5:R:550:4HP:H72	2.49	0.48
2:M:361:HIS:CG	4:M:601:BME:H21	2.48	0.48
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.96	0.47
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.14	0.47
2:N:497:ASN:HD22	2:N:497:ASN:C	2.21	0.47
1:F:54:GLN:HG3	1:F:184:ARG:HH21	1.79	0.47
1:D:163:GLN:HB3	1:D:165:GLN:HE22	1.79	0.47
1:A:100:ASP:OD1	1:A:100:ASP:N	2.41	0.47
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.44	0.47
1:B:69:GLU:HG2	1:B:94:ARG:HG2	1.95	0.47
1:D:5:LEU:O	2:P:387:GLN:HG2	2.14	0.47
1:F:80:GLN:O	1:F:91:SER:HB2	2.14	0.47
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.50	0.47
1:B:100:ASP:CG	1:B:101:ALA:H	2.22	0.47
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.49	0.47
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.47
2:P:307:ARG:CG	2:P:533:THR:HG22	2.42	0.47
2:P:449:TRP:CE3	5:P:550:4HP:H72	2.50	0.47
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.13	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.15	0.47
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.96	0.47
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.49	0.47
2:P:497:ASN:HD22	2:P:498:PRO:N	2.12	0.47
2:R:306:SER:CB	2:R:530:GLN:HE21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLU:CG	1:B:180:LYS:N	2.77	0.47
1:A:20:GLY:C	1:A:21:LEU:HD23	2.40	0.47
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.79	0.47
2:P:359:HIS:O	2:P:366:ASN:HB3	2.15	0.47
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.48	0.47
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.11	0.47
1:A:163:GLN:HB2	6:A:269:HOH:O	2.16	0.46
1:D:51:LEU:O	1:D:105:THR:HA	2.15	0.46
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.45	0.46
1:F:98:THR:HB	1:F:100:ASP:CG	2.40	0.46
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.31	0.46
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.42	0.46
1:C:99:PHE:CE2	2:O:411:LYS:HD2	2.49	0.46
1:E:38:ARG:HG3	1:E:107:HIS:HB2	1.97	0.46
1:F:64:ARG:O	1:F:99:PHE:HD1	1.98	0.46
2:M:438:SER:O	4:M:601:BME:H22	2.16	0.46
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.98	0.46
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.62	0.46
2:R:399:MET:HA	2:R:462:HIS:O	2.16	0.46
1:C:143:LEU:HD23	1:C:143:LEU:C	2.41	0.46
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.87	0.46
1:E:50:LEU:O	1:E:182:ALA:HA	2.16	0.46
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.98	0.46
1:F:176:GLU:OE2	1:F:179:GLY:C	2.58	0.46
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.97	0.46
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.50	0.46
1:C:100:ASP:CG	1:C:101:ALA:H	2.23	0.46
1:E:41:LYS:HZ2	1:E:86:GLU:C	2.23	0.46
2:R:356:PHE:CD2	2:R:428:ARG:HD3	2.51	0.46
1:B:50:LEU:O	1:B:182:ALA:HA	2.16	0.46
1:A:176:GLU:HG3	1:A:180:LYS:C	2.40	0.45
2:O:505:ILE:HG22	2:O:507:LYS:HE2	1.98	0.45
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.46	0.45
1:F:52:LEU:C	1:F:52:LEU:CD2	2.89	0.45
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.98	0.45
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.45	0.45
2:O:363:LEU:HD11	2:O:427:GLY:HA3	1.99	0.45
1:E:44:ALA:O	1:E:48:HIS:NE2	2.29	0.45
2:N:400:TRP:HA	2:N:425:GLY:O	2.16	0.45
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.97	0.45
1:F:174:ARG:HE	1:F:181:THR:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:CG	1:A:37:ASN:H	2.33	0.45
2:M:522:ARG:NE	2:M:524:ASP:OD1	2.47	0.45
2:N:416:LEU:C	2:N:416:LEU:CD2	2.90	0.45
1:E:98:THR:HG1	1:E:103:GLU:H	1.64	0.45
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.79	0.45
1:E:147:ASP:OD2	1:E:174:ARG:NH1	2.49	0.45
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.98	0.45
1:F:40:ALA:HB2	1:F:89:PHE:HD1	1.81	0.45
2:N:414:ARG:NE	2:N:414:ARG:CA	2.80	0.45
1:B:163:GLN:C	1:B:165:GLN:HE22	2.24	0.45
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.83	0.45
2:P:503:GLN:HG2	6:P:648:HOH:O	2.17	0.45
1:C:63:VAL:HG12	1:C:66:SER:HB3	1.98	0.45
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	3.05	0.45
1:A:165:GLN:NE2	1:C:61:HIS:NE2	2.65	0.45
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.51	0.45
1:C:98:THR:HB	1:C:100:ASP:CG	2.42	0.45
1:D:164:PRO:N	1:D:165:GLN:NE2	2.65	0.45
1:E:19:ILE:HD11	2:Q:408:TYR:HD2	1.82	0.45
2:O:400:TRP:HA	2:O:425:GLY:O	2.17	0.45
2:R:386:ASP:HA	2:R:527:LEU:O	2.17	0.45
2:R:437:TYR:CD1	2:R:437:TYR:C	2.94	0.45
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.97	0.44
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.99	0.44
1:C:191:GLY:O	1:C:194:GLU:HB2	2.17	0.44
1:D:50:LEU:O	1:D:182:ALA:HA	2.17	0.44
1:A:114:VAL:HG23	1:A:122:MET:CE	2.48	0.44
1:B:39:LEU:HD11	1:B:93:GLY:HA3	2.00	0.44
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.80	0.44
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.17	0.44
1:F:163:GLN:CA	1:F:165:GLN:HE22	2.30	0.44
2:N:478:LEU:HD12	2:N:523:PHE:CG	2.52	0.44
2:O:364:LEU:HB2	2:O:440:ARG:HD3	1.99	0.44
2:Q:399:MET:HA	2:Q:462:HIS:O	2.17	0.44
1:D:58:GLY:HA2	1:D:190:GLN:HB3	1.99	0.44
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.99	0.44
1:A:4:LEU:HB3	2:M:387:GLN:HB3	2.00	0.44
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.82	0.44
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.66	0.44
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.47	0.44
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:H	1:E:165:GLN:HE21	0.65	0.44
1:F:133:ARG:HG3	2:R:326:THR:HG21	1.99	0.44
1:F:177:VAL:O	1:F:180:LYS:HB3	2.17	0.44
2:M:335:ALA:HB1	2:O:325:LYS:HD3	2.00	0.44
1:F:157:VAL:O	1:F:160:LEU:HB2	2.18	0.44
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.52	0.44
2:P:447:TYR:HA	2:P:448:PRO:HD3	1.88	0.43
1:E:52:LEU:HA	1:E:104:TRP:O	2.18	0.43
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.53	0.43
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.89	0.43
2:P:489:CYS:C	2:P:493:LYS:HE3	2.43	0.43
2:R:376:GLU:O	2:R:442:ILE:HA	2.18	0.43
2:R:434:ASP:HB3	2:R:436:TYR:HD2	1.83	0.43
1:A:52:LEU:C	1:A:52:LEU:HD22	2.43	0.43
1:A:131:PHE:CE2	2:M:475:ILE:HD12	2.53	0.43
2:M:400:TRP:HA	2:M:425:GLY:O	2.18	0.43
2:O:361:HIS:CD2	6:O:708:HOH:O	2.71	0.43
2:O:392:VAL:HG12	2:O:395:THR:HB	2.01	0.43
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.18	0.43
2:Q:478:LEU:HD12	2:Q:523:PHE:CD2	2.53	0.43
2:M:399:MET:HA	2:M:462:HIS:O	2.18	0.43
2:P:505:ILE:HG22	2:P:507:LYS:HE3	2.01	0.43
1:A:199:ASP:O	2:M:338:SER:HA	2.19	0.43
2:O:413:ASP:C	2:O:414:ARG:HD2	2.44	0.43
1:C:132:ALA:HB3	1:C:135:ILE:HD12	2.00	0.43
1:E:115:ASN:HA	1:E:121:PRO:HA	2.01	0.43
2:R:497:ASN:HA	2:R:498:PRO:HD2	1.77	0.43
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.87	0.43
1:D:84:ASN:O	1:D:87:ASN:HB2	2.19	0.43
1:E:64:ARG:O	1:E:99:PHE:HD1	2.01	0.43
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.95	0.43
2:Q:478:LEU:HD12	2:Q:523:PHE:CG	2.54	0.43
1:F:4:LEU:HB3	2:R:387:GLN:HB3	2.01	0.43
2:N:307:ARG:HG2	2:N:533:THR:HG22	2.00	0.43
1:E:100:ASP:CG	1:E:101:ALA:N	2.72	0.43
2:P:361:HIS:CD2	2:P:361:HIS:N	2.83	0.43
2:P:399:MET:HA	2:P:462:HIS:O	2.19	0.43
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.77	0.43
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.19	0.43
2:M:359:HIS:O	2:M:366:ASN:HB3	2.19	0.42
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:O	1:B:102:GLY:HA2	2.20	0.42
2:O:361:HIS:H	2:O:361:HIS:HD2	1.62	0.42
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.88	0.42
1:A:49:ILE:C	1:A:180:LYS:HE2	2.45	0.42
2:M:361:HIS:CD2	2:M:361:HIS:N	2.71	0.42
2:M:516:MET:HE3	2:M:516:MET:HB3	1.78	0.42
2:P:478:LEU:C	2:P:478:LEU:CD2	2.87	0.42
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.18	0.42
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.54	0.42
2:P:392:VAL:HG12	2:P:395:THR:HB	2.01	0.42
1:E:168:GLU:CA	1:E:171:ILE:HD12	2.39	0.42
1:F:200:PHE:CD1	2:R:345:GLU:HG2	2.54	0.42
2:R:484:PRO:O	2:R:488:MET:CE	2.65	0.42
2:P:516:MET:HE3	2:P:516:MET:HB3	1.84	0.42
2:O:437:TYR:CD2	2:O:437:TYR:C	2.97	0.42
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.42
6:F:1371:HOH:O	2:R:301:PRO:HB2	2.19	0.42
1:A:100:ASP:CG	1:A:101:ALA:N	2.76	0.42
2:M:328:ILE:HD12	2:N:335:ALA:HB2	2.02	0.42
2:N:536:GLU:HB2	6:N:703:HOH:O	2.19	0.42
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.55	0.42
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.50	0.42
1:D:70:VAL:HG11	1:D:106:LEU:CD2	2.49	0.42
1:D:172:ALA:HB1	1:D:183:TYR:HB3	2.01	0.42
2:Q:493:LYS:HE3	2:Q:493:LYS:HB2	1.81	0.42
2:R:447:TYR:OH	5:R:550:4HP:C5	2.68	0.42
2:M:488:MET:CE	2:P:508:LEU:HD23	2.50	0.42
1:C:176:GLU:HG3	1:C:180:LYS:O	2.20	0.42
2:P:356:PHE:CD2	2:P:428:ARG:HD3	2.54	0.42
2:P:363:LEU:HD23	2:P:425:GLY:HA2	2.02	0.42
2:R:348:GLY:HA3	6:R:1270:HOH:O	2.19	0.42
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.85	0.42
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.54	0.41
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.55	0.41
2:Q:486:ILE:N	2:Q:487:PRO:CD	2.83	0.41
2:O:362:ASP:OD1	2:O:364:LEU:HB2	2.21	0.41
2:O:383:ARG:HA	2:O:435:GLY:O	2.20	0.41
2:P:307:ARG:HA	2:P:307:ARG:HD3	1.88	0.41
2:P:473:LYS:HE3	2:P:475:ILE:HG13	2.02	0.41
2:P:486:ILE:HB	2:P:487:PRO:HD3	2.02	0.41
2:M:497:ASN:ND2	2:M:499:GLU:N	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:486:ILE:N	2:O:487:PRO:CD	2.83	0.41
1:B:66:SER:HB2	1:B:130:LEU:HD11	2.01	0.41
1:B:163:GLN:HA	1:B:164:PRO:HD2	1.64	0.41
1:F:120:VAL:HA	1:F:121:PRO:HD2	1.89	0.41
1:A:92:PHE:CD1	2:M:349:PRO:HG3	2.56	0.41
1:A:110:LYS:NZ	1:A:148:GLU:OE2	2.44	0.41
2:M:416:LEU:C	2:M:416:LEU:CD2	2.92	0.41
1:C:114:VAL:CG2	1:C:122:MET:HE3	2.48	0.41
2:P:484:PRO:O	2:P:488:MET:CE	2.67	0.41
2:Q:392:VAL:HG12	2:Q:395:THR:HB	2.03	0.41
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.95	0.41
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.75	0.41
1:F:31:ARG:HH12	2:R:428:ARG:HG2	1.84	0.41
2:R:312:ASP:OD1	2:R:312:ASP:C	2.63	0.41
2:R:416:LEU:HD23	2:R:417:ALA:N	2.36	0.41
1:C:64:ARG:HB3	1:C:99:PHE:HA	2.03	0.41
1:E:19:ILE:HG21	1:E:19:ILE:HD13	1.74	0.41
1:F:146:ASP:OD1	1:F:174:ARG:HB2	2.20	0.41
2:R:517:ASP:C	2:R:517:ASP:OD1	2.62	0.41
2:M:486:ILE:N	2:M:487:PRO:HD2	2.36	0.41
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.36	0.41
2:N:361:HIS:H	2:N:361:HIS:HD2	1.69	0.41
2:N:497:ASN:HD22	2:N:498:PRO:N	2.19	0.41
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.02	0.41
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.56	0.41
1:C:52:LEU:HA	1:C:104:TRP:O	2.21	0.41
1:D:28:ASN:HB3	1:D:29:PRO:HD2	2.03	0.41
2:Q:480:PHE:O	2:Q:481:GLU:C	2.64	0.41
2:R:315:TRP:HE1	2:R:503:GLN:HE22	1.69	0.41
2:R:405:GLY:HA3	6:R:1275:HOH:O	2.21	0.41
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.72	0.41
2:M:486:ILE:HB	2:M:487:PRO:HD3	2.02	0.41
2:O:331:SER:HA	2:O:332:PRO:HD3	1.98	0.41
2:O:373:PRO:HB3	2:O:423:PHE:HB2	2.03	0.41
1:D:176:GLU:CG	1:D:179:GLY:HA2	2.51	0.41
1:F:177:VAL:N	1:F:180:LYS:O	2.40	0.41
2:M:447:TYR:OH	5:M:550:4HP:C5	2.69	0.40
2:M:448:PRO:CB	2:P:516:MET:HA	2.51	0.40
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.57	0.40
2:O:359:HIS:O	2:O:366:ASN:HB3	2.21	0.40
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:443:LYS:HE3	2:P:480:PHE:CG	2.56	0.40
2:P:465:ILE:HG12	2:P:525:ILE:HD13	2.03	0.40
1:C:144:TYR:CE1	1:C:158:LEU:HD13	2.56	0.40
2:O:484:PRO:O	2:O:488:MET:HE3	2.21	0.40
1:A:191:GLY:O	1:A:194:GLU:HB2	2.21	0.40
2:N:505:ILE:O	2:N:507:LYS:HE3	2.22	0.40
2:O:495:ILE:HG21	2:O:500:ALA:HB3	2.02	0.40
2:R:326:THR:HG22	2:R:330:ARG:HD2	2.04	0.40
1:B:23:LEU:HD12	1:B:23:LEU:N	2.36	0.40
2:P:522:ARG:NE	2:P:524:ASP:OD1	2.49	0.40
1:F:98:THR:OG1	1:F:101:ALA:HB3	2.21	0.40
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.22	0.40
1:E:78:GLU:OE1	6:E:239:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	194 (98%)	4 (2%)	0	100	100
1	B	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	193 (98%)	4 (2%)	1 (0%)	24	16
1	E	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
All	All	2562/2628 (98%)	2484 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	100	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	156 (96%)	6 (4%)	30	20
1	B	162/163 (99%)	152 (94%)	10 (6%)	16	6
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	15
1	D	162/163 (99%)	156 (96%)	6 (4%)	30	20
1	E	162/163 (99%)	155 (96%)	7 (4%)	26	15
1	F	162/163 (99%)	157 (97%)	5 (3%)	35	26
2	M	196/202 (97%)	182 (93%)	14 (7%)	13	4
2	N	196/202 (97%)	185 (94%)	11 (6%)	19	8
2	O	196/202 (97%)	185 (94%)	11 (6%)	19	8
2	P	196/202 (97%)	188 (96%)	8 (4%)	27	17
2	Q	196/202 (97%)	189 (96%)	7 (4%)	31	21
2	R	196/202 (97%)	187 (95%)	9 (5%)	24	13
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	23	12

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	19	ILE
1	A	38	ARG
1	A	52	LEU
1	A	143	LEU
1	A	165	GLN
2	M	364	LEU
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	442	ILE
2	M	478	LEU
2	M	488	MET
2	M	497	ASN
2	M	503	GLN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	38	ARG
1	B	52	LEU
1	B	106	LEU
1	B	143	LEU
1	B	158	LEU
1	B	165	GLN
1	B	176	GLU
1	B	180	LYS
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	416	LEU
2	N	433	SER
2	N	442	ILE
2	N	478	LEU
2	N	497	ASN
2	N	499	GLU
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE

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Mol	Chain	Res	Type
1	C	38	ARG
1	C	47	GLU
1	C	52	LEU
1	C	94	ARG
1	C	165	GLN
2	O	364	LEU
2	O	372	LEU
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	434	ASP
2	O	473	LYS
2	O	478	LEU
2	O	503	GLN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	395	THR
2	P	411	LYS
2	P	416	LEU
2	P	434	ASP
2	P	440	ARG
2	P	442	ILE
2	P	478	LEU
1	E	4	LEU
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU
1	E	114	VAL
1	E	165	GLN
1	E	180	LYS
2	Q	364	LEU
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG

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Mol	Chain	Res	Type
2	Q	434	ASP
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	38	ARG
1	F	52	LEU
1	F	165	GLN
2	R	364	LEU
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP
2	R	478	LEU
2	R	497	ASN
2	R	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	165	GLN
2	M	361	HIS
2	M	497	ASN
2	M	502	GLN
1	B	165	GLN
2	N	334	GLN
2	N	412	ASN
2	N	497	ASN
1	C	11	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	59	ASN
1	D	127	ASN
1	D	163	GLN
1	D	165	GLN
2	P	359	HIS
2	P	361	HIS
2	P	394	ASN

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Mol	Chain	Res	Type
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
2	P	514	ASN
2	P	530	GLN
1	E	163	GLN
1	E	165	GLN
2	Q	334	GLN
2	Q	361	HIS
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	140	HIS
1	F	165	GLN
2	R	361	HIS
2	R	394	ASN
2	R	412	ASN
2	R	422	ASN
2	R	497	ASN
2	R	502	GLN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BME	M	601	2	3,3,3	0.92	0	2,2,2	0.94	0
4	BME	P	601	2	3,3,3	0.42	0	2,2,2	0.56	0
4	BME	N	601	2	3,3,3	0.15	0	2,2,2	0.07	0
5	4HP	N	550	3	11,11,11	1.36	2 (18%)	14,14,14	0.98	1 (7%)
5	4HP	R	550	3	11,11,11	1.06	0	14,14,14	0.78	0
5	4HP	M	550	3	11,11,11	1.23	1 (9%)	14,14,14	1.00	0
4	BME	Q	601	2	3,3,3	0.68	0	2,2,2	0.32	0
5	4HP	O	550	3	11,11,11	1.30	2 (18%)	14,14,14	0.83	0
5	4HP	Q	550	3	11,11,11	1.30	2 (18%)	14,14,14	1.18	2 (14%)
5	4HP	P	550	3	11,11,11	1.23	0	14,14,14	1.04	1 (7%)
4	BME	R	601	2	3,3,3	0.64	0	2,2,2	1.20	0
4	BME	O	601	2	3,3,3	0.41	0	2,2,2	0.09	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
4	BME	M	601	2	-	0/1/1/1	-
4	BME	P	601	2	-	0/1/1/1	-
4	BME	N	601	2	-	1/1/1/1	-
5	4HP	N	550	3	-	0/4/4/4	0/1/1/1
5	4HP	R	550	3	-	0/4/4/4	0/1/1/1
5	4HP	M	550	3	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	-
5	4HP	O	550	3	-	0/4/4/4	0/1/1/1
5	4HP	Q	550	3	-	0/4/4/4	0/1/1/1
5	4HP	P	550	3	-	0/4/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	-
4	BME	O	601	2	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	550	4HP	C2-C1	2.74	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	4HP	C7-C1	2.39	1.55	1.51
5	M	550	4HP	C7-C8	2.32	1.56	1.51
5	Q	550	4HP	C7-C8	2.25	1.55	1.51
5	N	550	4HP	C7-C8	2.20	1.55	1.51
5	O	550	4HP	C7-C8	2.18	1.55	1.51
5	O	550	4HP	O2-C8	-2.07	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	550	4HP	C5-C6-C1	-2.23	118.06	121.00
5	P	550	4HP	C7-C1-C2	-2.05	117.87	120.89
5	Q	550	4HP	C2-C3-C4	-2.00	117.76	119.88
5	N	550	4HP	C7-C1-C2	-2.00	117.94	120.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	601	BME	3	0
5	N	550	4HP	2	0
5	R	550	4HP	3	0
5	M	550	4HP	4	0
4	Q	601	BME	1	0
5	O	550	4HP	4	0
5	Q	550	4HP	2	0
5	P	550	4HP	5	0
4	O	601	BME	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.