



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:34 AM UTC

PDB ID : 3PCM / pdb_00003pcm
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 6-HYDROXYNICOTINIC ACID N-OXIDE AND CYANIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

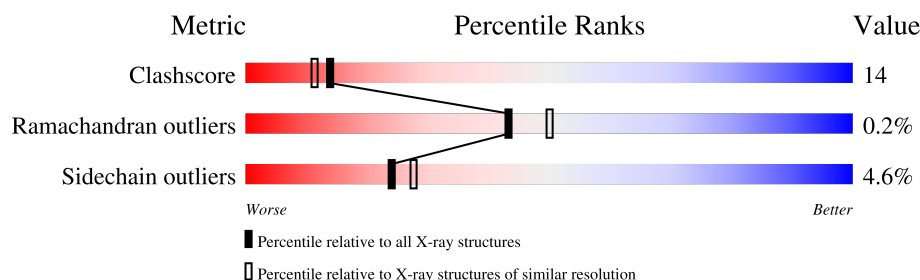
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	68% 27% .
1	B	200	73% 22% 5%
1	C	200	69% 27% .
1	D	200	66% 28% 6%
1	E	200	68% 29% .
1	F	200	61% 34% 5%
2	M	238	65% 29% . .
2	N	238	71% 22% 5% .

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Mol	Chain	Length	Quality of chain
2	O	238	68%24%5%•
2	P	238	64%26%8%•
2	Q	238	66%25%6%••
2	R	238	61%31%6%•

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21966 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.

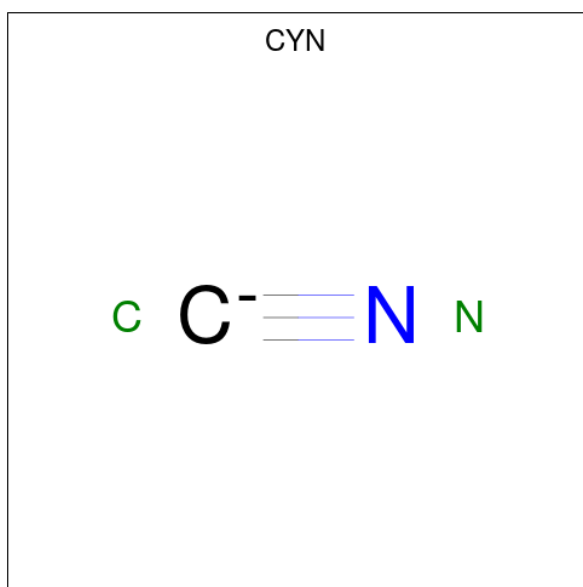
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 CYANIDE ION (CCD ID: CYN) (formula: CN).

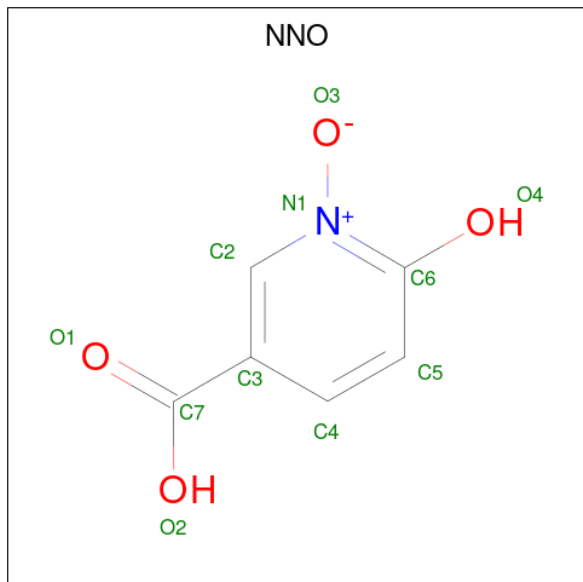


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

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

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

- Molecule 5 is 6-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: NNO) (formula: $C_6H_5NO_4$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	77	Total	O	0	0
			77	77		
6	M	154	Total	O	0	0
			154	154		
6	B	86	Total	O	0	0
			86	86		
6	N	156	Total	O	0	0
			156	156		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	78	Total 78	O 78	0	0
6	O	156	Total 156	O 156	0	0
6	D	80	Total 80	O 80	0	0
6	P	151	Total 151	O 151	0	0
6	E	79	Total 79	O 79	0	0
6	Q	161	Total 161	O 161	0	0
6	F	78	Total 78	O 78	0	0
6	R	160	Total 160	O 160	0	0

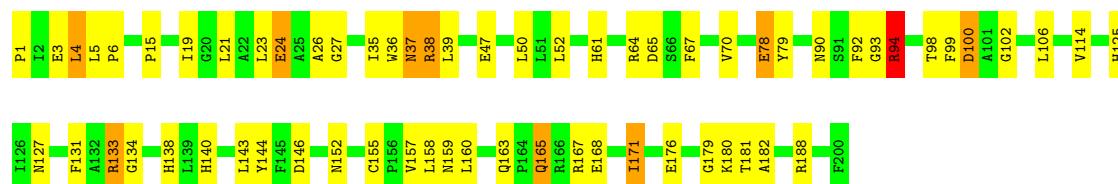
3 Residue-property plots [i](#)

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.

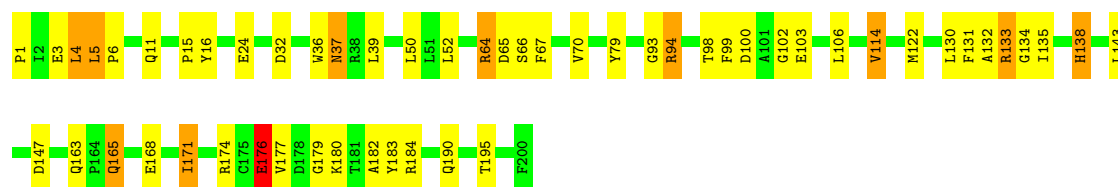
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



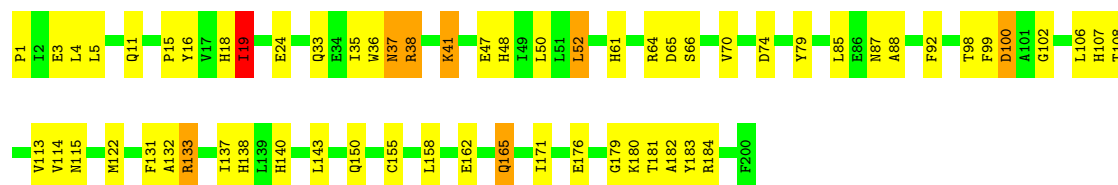
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



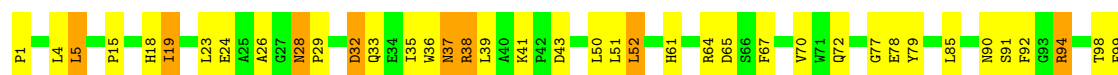
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



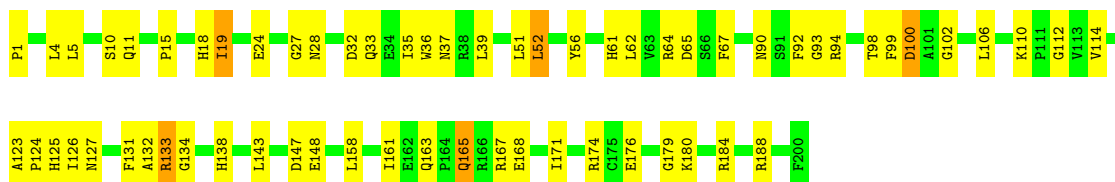
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 

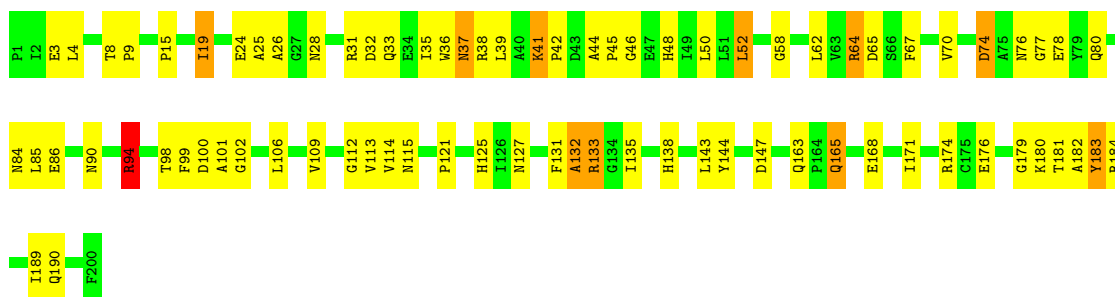




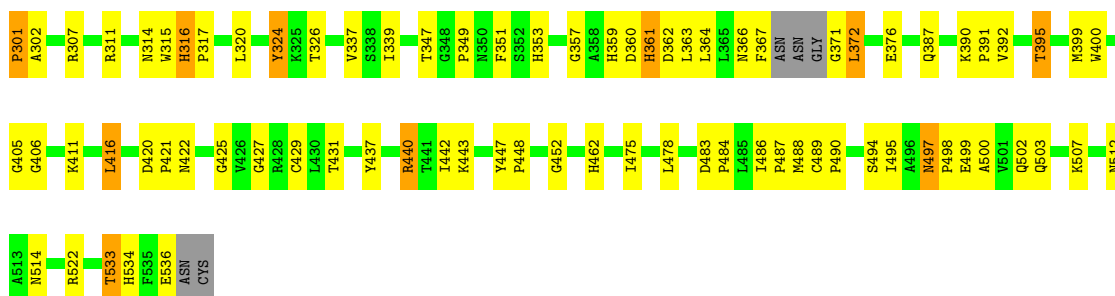
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



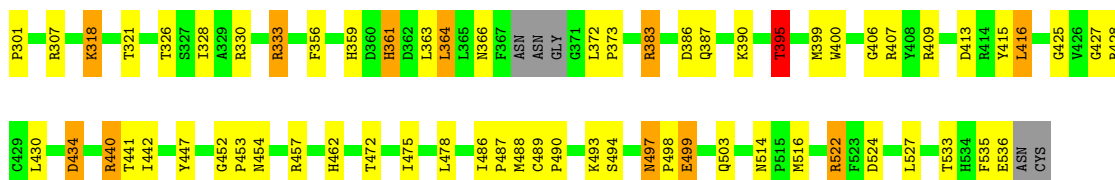
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

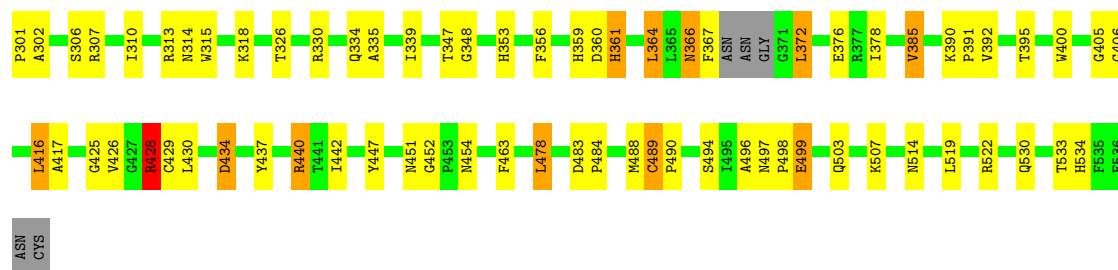


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



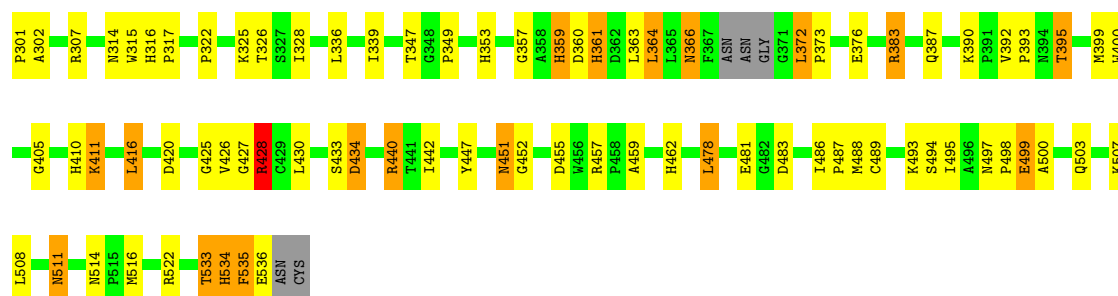
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:  68% 24% 5% .



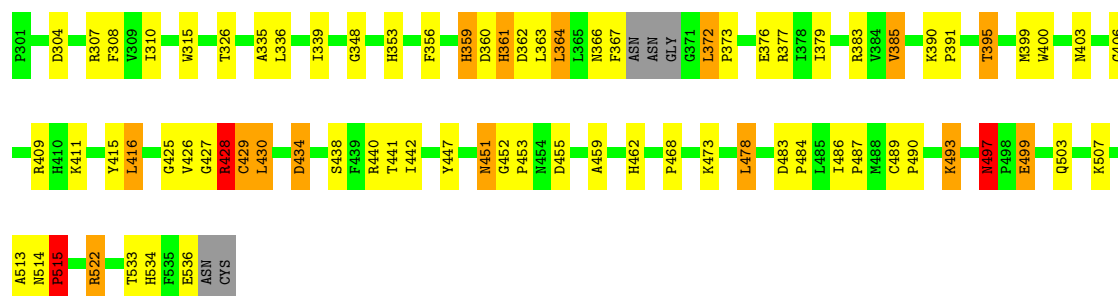
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:  64% 26% 8% .



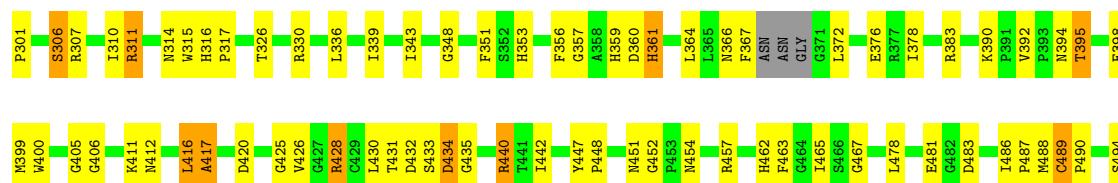
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:  66% 25% 6% ..



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:  61% 31% 6% .



I495	A496	N497	P498	E499	A500	Q503	M514	P515	M516	L519	R522	F523	D524	Q530	T533	H534	F535	E536	ASN	CYS
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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	196.10 Å 127.30 Å 134.50 Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.25	Depositor
% Data completeness (in resolution range)	91.0 (6.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21966	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: NNO, FE, CYN

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	1.11	1/1611 (0.1%)	1.73	20/2195 (0.9%)
1	B	1.11	1/1611 (0.1%)	1.70	17/2195 (0.8%)
1	C	1.12	1/1611 (0.1%)	1.68	19/2195 (0.9%)
1	D	1.10	0/1611	1.67	15/2195 (0.7%)
1	E	1.13	0/1611	1.62	10/2195 (0.5%)
1	F	1.20	1/1611 (0.1%)	1.75	20/2195 (0.9%)
2	M	1.19	0/1895	1.73	23/2580 (0.9%)
2	N	1.19	3/1895 (0.2%)	1.71	20/2580 (0.8%)
2	O	1.19	1/1895 (0.1%)	1.80	36/2580 (1.4%)
2	P	1.25	1/1895 (0.1%)	1.76	38/2580 (1.5%)
2	Q	1.28	4/1895 (0.2%)	1.79	34/2580 (1.3%)
2	R	1.25	2/1895 (0.1%)	1.78	35/2580 (1.4%)
All	All	1.18	15/21036 (0.1%)	1.73	287/28650 (1.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	9.36	1.56	1.52
2	P	451	ASN	CA-C	9.11	1.56	1.52
2	Q	451	ASN	CA-C	8.41	1.56	1.52
1	A	94	ARG	CD-NE	-6.88	1.36	1.46
2	Q	428	ARG	CD-NE	-6.10	1.37	1.46
2	Q	441	THR	CA-CB	5.86	1.61	1.54
1	B	94	ARG	CD-NE	-5.80	1.38	1.46
2	R	467	GLY	N-CA	5.61	1.52	1.44
2	N	441	THR	CA-CB	5.52	1.60	1.54
2	N	321	THR	N-CA	5.36	1.52	1.46
2	N	472	THR	CA-CB	5.34	1.62	1.53
1	F	135	ILE	CA-CB	5.23	1.59	1.53
2	Q	459	ALA	N-CA	5.20	1.52	1.46
1	C	108	THR	CA-CB	5.08	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	395	THR	N-CA	5.04	1.51	1.45

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	19.04	151.05	124.40
2	Q	428	ARG	CD-NE-CZ	12.42	141.79	124.40
2	O	451	ASN	O-C-N	10.95	128.93	120.83
2	O	428	ARG	CD-NE-CZ	10.82	139.55	124.40
2	N	452	GLY	N-CA-C	-10.73	99.25	112.23
2	P	452	GLY	N-CA-C	-10.47	99.22	112.10
1	F	94	ARG	NE-CZ-NH1	10.20	131.70	121.50
2	Q	452	GLY	N-CA-C	-10.18	99.91	112.23
2	Q	361	HIS	CA-CB-CG	-9.71	104.09	113.80
2	O	353	HIS	CA-CB-CG	-9.56	104.24	113.80
2	O	452	GLY	N-CA-C	-9.54	100.37	112.10
1	F	37	ASN	N-CA-C	9.02	122.53	112.97
2	R	361	HIS	CA-CB-CG	-8.96	104.84	113.80
2	Q	451	ASN	O-C-N	8.50	127.12	120.83
2	P	451	ASN	O-C-N	8.48	127.11	120.83
1	C	87	ASN	CA-CB-CG	8.48	121.08	112.60
1	D	37	ASN	N-CA-C	8.42	122.36	112.93
2	O	434	ASP	CA-CB-CG	-8.34	104.26	112.60
1	F	127	ASN	CA-CB-CG	-8.25	104.35	112.60
1	D	38	ARG	CD-NE-CZ	-8.24	112.86	124.40
2	P	372	LEU	CB-CA-C	8.12	119.89	108.76
2	M	353	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	47	GLU	CB-CG-CD	7.95	126.12	112.60
2	P	420	ASP	CB-CA-C	7.92	119.26	110.15
1	F	90	ASN	CA-CB-CG	7.89	120.49	112.60
2	P	440	ARG	NE-CZ-NH2	-7.89	112.10	119.20
2	R	434	ASP	CA-CB-CG	-7.87	104.73	112.60
1	A	146	ASP	CA-CB-CG	7.79	120.39	112.60
2	O	440	ARG	CD-NE-CZ	-7.79	113.50	124.40
2	Q	377	ARG	CD-NE-CZ	-7.77	113.52	124.40
1	D	171	ILE	N-CA-C	7.75	119.05	107.51
2	R	392	VAL	O-C-N	7.73	128.38	120.96
1	C	115	ASN	CA-CB-CG	7.64	120.24	112.60
2	N	361	HIS	CA-CB-CG	-7.49	106.31	113.80
1	D	100	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	37	ASN	N-CA-C	7.47	120.89	112.97
1	D	186	ASP	CA-CB-CG	7.40	120.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	339	ILE	O-C-N	7.33	126.31	121.69
1	B	5	LEU	N-CA-C	-7.23	100.10	110.08
1	A	5	LEU	N-CA-C	-7.22	100.66	109.83
1	C	37	ASN	N-CA-C	7.17	121.68	113.15
2	R	481	GLU	CB-CG-CD	7.16	124.77	112.60
2	Q	514	ASN	O-C-N	7.13	127.90	121.19
2	M	494	SER	N-CA-C	-7.13	103.68	112.38
2	R	314	ASN	N-CA-C	-7.10	104.49	113.72
1	C	41	LYS	N-CA-C	-7.09	101.13	109.93
2	N	440	ARG	NE-CZ-NH2	-7.05	112.86	119.20
1	B	94	ARG	NE-CZ-NH2	-7.04	112.86	119.20
1	E	5	LEU	N-CA-C	-7.03	101.21	109.93
1	D	94	ARG	NE-CZ-NH2	-7.00	112.90	119.20
2	R	454	ASN	CA-CB-CG	6.96	119.56	112.60
2	R	353	HIS	CA-CB-CG	-6.91	106.89	113.80
2	P	511	ASN	CA-CB-CG	6.88	119.48	112.60
1	B	37	ASN	N-CA-C	6.87	120.63	112.93
2	N	494	SER	N-CA-C	-6.87	103.81	111.71
1	E	125	HIS	CA-CB-CG	-6.79	107.01	113.80
2	R	392	VAL	CA-C-O	-6.77	116.28	120.88
2	N	428	ARG	CD-NE-CZ	6.77	133.88	124.40
2	P	361	HIS	CA-CB-CG	-6.73	107.07	113.80
2	M	443	LYS	O-C-N	6.72	127.43	121.18
2	M	361	HIS	CA-CB-CG	-6.68	107.12	113.80
2	Q	428	ARG	CG-CD-NE	6.62	126.58	112.00
2	M	440	ARG	CD-NE-CZ	-6.61	115.15	124.40
1	B	94	ARG	CG-CD-NE	6.60	126.51	112.00
1	B	176	GLU	CB-CG-CD	6.59	123.80	112.60
2	O	361	HIS	CA-CB-CG	-6.58	107.22	113.80
1	B	177	VAL	CB-CA-C	6.54	119.25	110.42
2	R	457	ARG	CD-NE-CZ	6.54	133.55	124.40
2	Q	348	GLY	O-C-N	6.53	128.30	121.77
2	O	334	GLN	OE1-CD-NE2	-6.47	116.13	122.60
1	F	94	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	C	133	ARG	CA-CB-CG	6.45	127.00	114.10
2	O	451	ASN	CA-C-O	-6.44	116.10	119.77
2	Q	430	LEU	N-CA-CB	-6.43	100.15	110.63
2	M	514	ASN	O-C-N	6.43	127.23	121.19
1	F	133	ARG	N-CA-C	-6.43	101.18	110.24
2	P	314	ASN	N-CA-C	-6.41	105.61	113.50
2	P	494	SER	N-CA-C	-6.40	104.74	112.54
1	D	178	ASP	CA-CB-CG	-6.39	106.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	428	ARG	CG-CD-NE	6.39	126.07	112.00
2	P	383	ARG	CD-NE-CZ	-6.38	115.46	124.40
2	O	428	ARG	CG-CD-NE	6.36	126.00	112.00
2	N	475	ILE	N-CA-CB	6.32	120.13	111.41
1	F	94	ARG	CD-NE-CZ	6.28	133.19	124.40
2	O	514	ASN	CA-CB-CG	6.27	118.87	112.60
1	E	112	GLY	CA-C-N	6.18	129.50	120.91
1	E	112	GLY	C-N-CA	6.18	129.50	120.91
2	O	417	ALA	N-CA-C	-6.17	102.28	109.93
2	P	339	ILE	O-C-N	6.17	125.58	121.69
2	P	428	ARG	NE-CZ-NH1	6.17	127.67	121.50
2	R	412	ASN	CA-CB-CG	6.16	118.76	112.60
1	A	38	ARG	CD-NE-CZ	-6.15	115.79	124.40
2	R	463	PHE	CA-CB-CG	6.15	119.95	113.80
1	B	94	ARG	NE-CZ-NH1	6.11	127.61	121.50
2	N	409	ARG	NE-CZ-NH2	6.09	124.69	119.20
1	F	38	ARG	CD-NE-CZ	-6.08	115.89	124.40
2	P	353	HIS	CA-CB-CG	-6.08	107.72	113.80
1	A	152	ASN	CA-CB-CG	6.07	118.67	112.60
2	R	494	SER	N-CA-C	-6.07	105.14	112.54
2	O	314	ASN	CB-CA-C	6.07	120.20	109.65
1	E	133	ARG	CA-CB-CG	6.06	126.22	114.10
1	C	47	GLU	CB-CG-CD	6.05	122.89	112.60
2	O	494	SER	N-CA-C	-6.05	105.16	112.54
1	C	48	HIS	CA-CB-CG	-6.04	107.76	113.80
2	M	314	ASN	N-CA-C	-6.03	105.97	113.38
1	E	28	ASN	O-C-N	6.03	126.62	121.20
2	R	483	ASP	CB-CA-C	6.03	119.57	109.69
1	B	64	ARG	CD-NE-CZ	-6.01	115.98	124.40
2	Q	377	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	167	ARG	CD-NE-CZ	-5.99	116.01	124.40
2	P	459	ALA	N-CA-C	-5.99	101.55	110.23
2	N	454	ASN	CA-CB-CG	5.98	118.58	112.60
1	D	5	LEU	N-CA-C	-5.98	102.24	109.83
2	O	499	GLU	CB-CG-CD	5.96	122.73	112.60
1	A	140	HIS	CA-CB-CG	5.95	119.75	113.80
2	Q	360	ASP	CB-CA-C	5.95	120.67	110.79
2	P	314	ASN	N-CA-CB	5.95	119.28	110.53
1	F	46	GLY	CA-C-O	-5.94	118.17	122.45
2	N	409	ARG	NE-CZ-NH1	-5.92	115.58	121.50
2	M	452	GLY	N-CA-C	-5.91	100.28	112.34
2	R	457	ARG	CA-CB-CG	5.88	125.85	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	183	TYR	CA-CB-CG	5.86	124.45	113.90
2	P	357	GLY	N-CA-C	-5.85	105.89	112.33
1	C	181	THR	N-CA-CB	5.83	118.69	109.71
2	O	496	ALA	CA-C-O	-5.82	113.28	119.97
1	D	127	ASN	CA-CB-CG	-5.82	106.78	112.60
1	A	94	ARG	NE-CZ-NH1	5.80	127.30	121.50
2	P	428	ARG	CB-CG-CD	5.80	124.64	111.30
2	O	366	ASN	N-CA-C	5.79	120.21	113.20
2	P	430	LEU	N-CA-CB	-5.79	101.48	110.57
1	E	127	ASN	CA-CB-CG	-5.79	106.81	112.60
2	O	489	CYS	N-CA-C	5.79	117.98	109.42
2	M	357	GLY	N-CA-C	-5.78	105.14	112.54
2	P	457	ARG	CD-NE-CZ	5.77	132.48	124.40
2	P	410	HIS	CA-C-N	5.77	129.47	120.82
2	P	410	HIS	C-N-CA	5.77	129.47	120.82
1	C	183	TYR	N-CA-CB	5.77	119.82	110.77
1	B	133	ARG	CA-CB-CG	5.76	125.63	114.10
1	B	138	HIS	CA-CB-CG	-5.76	108.04	113.80
2	N	395	THR	CA-CB-OG1	-5.76	100.97	109.60
2	P	322	PRO	N-CA-C	5.76	122.16	113.81
1	B	94	ARG	CB-CG-CD	5.75	124.52	111.30
2	O	533	THR	CA-CB-OG1	-5.72	101.01	109.60
2	P	447	TYR	N-CA-CB	-5.72	100.19	110.37
2	R	420	ASP	CB-CA-C	5.72	116.72	110.15
2	O	430	LEU	N-CA-CB	-5.71	100.90	110.83
2	M	411	LYS	CA-CB-CG	5.71	125.51	114.10
2	Q	441	THR	N-CA-CB	-5.71	102.41	110.51
1	A	100	ASP	CA-CB-CG	-5.70	106.90	112.60
2	M	502	GLN	OE1-CD-NE2	5.69	128.29	122.60
2	O	372	LEU	CB-CA-C	5.68	116.58	108.68
1	C	38	ARG	CD-NE-CZ	-5.68	116.45	124.40
2	R	417	ALA	N-CA-C	-5.68	102.62	109.83
1	B	133	ARG	N-CA-C	-5.66	102.02	110.23
2	O	514	ASN	OD1-CG-ND2	-5.65	116.95	122.60
2	O	463	PHE	CA-CB-CG	5.65	119.45	113.80
2	Q	359	HIS	CA-CB-CG	-5.65	108.15	113.80
2	R	489	CYS	CA-C-N	5.64	125.17	119.19
2	R	489	CYS	C-N-CA	5.64	125.17	119.19
2	Q	383	ARG	CD-NE-CZ	-5.62	116.53	124.40
2	N	514	ASN	O-C-N	5.62	126.53	120.85
2	N	522	ARG	CD-NE-CZ	5.62	132.26	124.40
2	Q	522	ARG	CD-NE-CZ	-5.61	116.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	GLN	N-CA-CB	5.61	121.95	111.52
2	M	324	TYR	CA-C-N	5.61	129.23	120.82
2	M	324	TYR	C-N-CA	5.61	129.23	120.82
2	M	311	ARG	CD-NE-CZ	5.60	132.24	124.40
1	D	41	LYS	N-CA-C	-5.58	102.59	110.29
2	Q	459	ALA	N-CA-C	-5.57	102.15	110.23
2	Q	452	GLY	CA-C-O	-5.57	116.64	122.38
1	A	171	ILE	N-CA-C	5.57	115.80	107.51
2	Q	385	VAL	CA-C-O	-5.56	116.00	121.67
2	O	307	ARG	N-CA-C	-5.56	100.72	109.50
1	C	150	GLN	CB-CG-CD	5.55	122.04	112.60
2	Q	434	ASP	CA-CB-CG	-5.54	107.06	112.60
2	Q	379	ILE	O-C-N	5.54	129.24	123.26
2	O	314	ASN	N-CA-C	-5.54	106.57	113.38
2	Q	411	LYS	CB-CA-C	-5.53	101.56	110.74
2	Q	497	ASN	CB-CA-C	5.52	117.33	109.38
2	R	392	VAL	N-CA-C	-5.52	102.68	108.15
2	M	320	LEU	O-C-N	5.52	129.62	123.05
2	Q	367	PHE	CA-C-O	-5.51	111.43	120.80
2	O	339	ILE	CB-CA-C	5.51	114.73	109.33
1	B	183	TYR	N-CA-CB	5.50	120.06	110.81
1	A	23	LEU	CB-CA-C	5.49	119.95	110.84
1	D	28	ASN	O-C-N	5.48	126.14	121.20
2	O	489	CYS	CA-C-N	5.48	125.31	119.28
2	O	489	CYS	C-N-CA	5.48	125.31	119.28
2	M	367	PHE	CA-C-O	-5.47	111.49	120.80
1	F	189	ILE	O-C-N	5.47	127.47	121.83
2	R	367	PHE	CA-C-O	-5.47	111.50	120.80
2	M	372	LEU	CB-CA-C	5.47	116.28	108.68
2	P	533	THR	CA-CB-OG1	-5.46	101.40	109.60
2	P	359	HIS	CA-CB-CG	-5.46	108.34	113.80
2	Q	409	ARG	NE-CZ-NH2	5.46	124.11	119.20
2	P	440	ARG	NH1-CZ-NH2	5.45	126.39	119.30
2	N	452	GLY	CA-C-O	-5.45	116.77	122.38
2	Q	339	ILE	O-C-N	5.44	125.12	121.69
2	R	533	THR	CA-CB-OG1	-5.42	101.47	109.60
2	R	514	ASN	CB-CA-C	5.41	115.52	110.17
2	Q	522	ARG	NE-CZ-NH1	-5.40	116.10	121.50
2	R	430	LEU	N-CA-CB	-5.40	102.00	110.69
2	R	357	GLY	N-CA-C	-5.40	106.39	112.33
2	R	339	ILE	O-C-N	5.39	125.09	121.69
1	D	199	ASP	CA-CB-CG	5.39	117.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CB-CG-CD	5.39	123.69	111.30
2	R	348	GLY	O-C-N	5.39	127.16	121.77
2	P	499	GLU	CA-CB-CG	5.37	124.84	114.10
1	F	181	THR	N-CA-CB	5.37	117.84	109.85
1	E	133	ARG	N-CA-C	-5.34	102.49	110.23
2	R	452	GLY	N-CA-C	-5.34	101.45	112.34
1	F	64	ARG	CD-NE-CZ	-5.33	116.94	124.40
2	N	514	ASN	CA-CB-CG	5.33	117.93	112.60
1	C	19	ILE	CA-CB-CG2	5.32	119.55	110.50
1	A	94	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	D	150	GLN	N-CA-CB	5.32	117.78	110.07
2	N	434	ASP	CA-CB-CG	-5.32	107.28	112.60
2	Q	353	HIS	CA-CB-CG	-5.32	108.48	113.80
2	P	336	LEU	CA-C-O	-5.31	115.77	121.56
2	M	431	THR	N-CA-C	-5.30	103.53	110.53
1	F	112	GLY	N-CA-C	-5.30	105.51	112.82
1	B	11	GLN	CA-C-O	-5.29	115.06	120.99
1	C	133	ARG	N-CA-C	-5.29	102.78	110.24
2	O	367	PHE	CA-C-O	-5.29	111.81	120.80
2	M	316	HIS	O-C-N	5.28	127.45	121.53
2	P	452	GLY	CA-C-O	-5.28	117.34	122.46
1	A	21	LEU	N-CA-C	5.27	120.57	113.72
2	O	392	VAL	O-C-N	5.27	127.11	121.10
1	E	90	ASN	CA-CB-CG	5.25	117.85	112.60
2	Q	372	LEU	CB-CA-C	5.25	116.71	108.63
1	F	125	HIS	CA-CB-CG	-5.25	108.55	113.80
2	Q	499	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	26	ALA	N-CA-C	-5.24	106.14	112.54
2	N	383	ARG	CD-NE-CZ	-5.24	117.06	124.40
2	O	454	ASN	CA-CB-CG	5.23	117.83	112.60
2	R	336	LEU	CA-C-O	-5.23	115.86	121.56
1	B	195	THR	CA-CB-OG1	-5.21	101.78	109.60
2	R	440	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	F	113	VAL	N-CA-CB	-5.21	103.12	110.26
2	P	393	PRO	CA-C-N	5.21	129.81	122.46
2	P	393	PRO	C-N-CA	5.21	129.81	122.46
1	F	41	LYS	N-CA-C	-5.21	103.51	110.07
2	N	333	ARG	N-CA-C	-5.19	107.33	113.97
2	P	514	ASN	CB-CA-C	5.19	115.11	110.44
2	P	411	LYS	CB-CA-C	-5.18	102.14	110.74
2	R	451	ASN	O-C-N	5.18	129.48	122.59
2	P	366	ASN	N-CA-C	5.18	119.22	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	ASN	OD1-CG-ND2	5.18	127.78	122.60
2	O	307	ARG	CA-C-O	-5.17	115.06	121.11
2	R	314	ASN	CB-CA-C	5.17	118.24	109.55
2	R	311	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	F	62	LEU	O-C-N	5.16	129.18	122.89
2	M	337	VAL	CA-C-O	-5.14	114.99	120.59
2	M	339	ILE	O-C-N	5.14	126.96	121.10
2	R	522	ARG	CD-NE-CZ	-5.14	117.21	124.40
1	C	162	GLU	N-CA-C	5.13	117.28	111.02
2	N	318	LYS	N-CA-C	-5.13	103.91	110.53
1	C	5	LEU	N-CA-C	-5.13	103.32	109.83
1	D	171	ILE	N-CA-CB	-5.12	105.01	111.41
1	A	133	ARG	N-CA-C	-5.12	102.47	110.10
1	C	137	ILE	CB-CA-C	5.12	117.81	110.33
1	F	28	ASN	O-C-N	5.12	125.80	121.20
2	P	366	ASN	CA-CB-CG	5.10	117.70	112.60
2	O	451	ASN	N-CA-C	-5.10	100.35	108.30
2	P	481	GLU	CB-CG-CD	5.09	121.25	112.60
1	F	74	ASP	CA-CB-CG	-5.09	107.51	112.60
1	C	140	HIS	CA-CB-CG	5.08	118.88	113.80
1	C	171	ILE	CB-CA-C	5.08	117.11	110.96
2	Q	403	ASN	CA-CB-CG	5.08	117.68	112.60
2	Q	336	LEU	CA-C-O	-5.07	116.03	121.56
2	N	524	ASP	O-C-N	5.06	128.91	123.10
2	R	536	GLU	CA-C-O	5.06	129.39	120.80
2	R	314	ASN	CA-CB-CG	5.05	117.65	112.60
2	Q	308	PHE	CB-CA-C	5.04	118.46	109.38
2	N	457	ARG	CB-CG-CD	5.04	122.89	111.30
2	Q	515	PRO	CA-C-O	-5.04	115.67	121.36
2	M	533	THR	N-CA-C	-5.04	103.40	110.50
2	O	348	GLY	O-C-N	5.04	126.81	121.77
2	Q	468	PRO	N-CA-C	5.03	120.15	113.86
1	B	4	LEU	N-CA-CB	-5.03	100.97	110.07
1	A	90	ASN	CA-CB-CG	5.03	117.63	112.60
1	D	32	ASP	O-C-N	5.03	127.46	122.08
1	B	171	ILE	N-CA-C	5.03	115.00	107.51
2	M	411	LYS	CB-CA-C	-5.02	100.43	110.42
1	A	125	HIS	CA-CB-CG	-5.01	108.79	113.80
2	O	385	VAL	CA-C-O	-5.00	116.57	121.67
2	P	314	ASN	CB-CA-C	5.00	118.39	109.29

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	41	0
1	C	1571	0	1499	43	0
1	D	1571	0	1499	55	0
1	E	1571	0	1499	55	0
1	F	1571	0	1499	61	0
2	M	1840	0	1794	58	0
2	N	1840	0	1794	52	0
2	O	1840	0	1794	51	0
2	P	1840	0	1794	57	0
2	Q	1840	0	1794	60	0
2	R	1840	0	1794	61	0
3	M	2	0	0	1	0
3	N	2	0	0	0	0
3	O	2	0	0	1	0
3	P	2	0	0	1	0
3	Q	2	0	0	1	0
3	R	2	0	0	1	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	M	11	0	3	1	0
5	N	11	0	3	0	0
5	O	11	0	3	0	0
5	P	11	0	3	0	0
5	Q	11	0	3	0	0
5	R	11	0	3	0	0
6	A	77	0	0	1	0
6	B	86	0	0	0	0
6	C	78	0	0	0	0
6	D	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	79	0	0	3	0
6	F	78	0	0	0	0
6	M	154	0	0	7	0
6	N	156	0	0	4	0
6	O	156	0	0	4	0
6	P	151	0	0	7	0
6	Q	161	0	0	5	0
6	R	160	0	0	5	0
All	All	21966	0	19776	582	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 (582) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLN:H	1:B:165:GLN:NE2	1.49	1.09
1:C:64:ARG:NH1	1:C:100:ASP:O	1.92	1.02
1:F:64:ARG:NH1	1:F:100:ASP:O	1.92	1.00
1:B:165:GLN:HE21	1:B:165:GLN:N	1.59	1.00
1:D:64:ARG:NH1	1:D:100:ASP:O	1.93	1.00
1:F:165:GLN:H	1:F:165:GLN:NE2	1.68	0.91
2:N:390:LYS:HE2	6:N:723:HOH:O	1.69	0.91
2:N:390:LYS:HD3	6:N:647:HOH:O	1.73	0.88
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.56	0.88
2:R:497:ASN:HD22	2:R:499:GLU:H	1.22	0.88
1:A:64:ARG:NH1	1:A:100:ASP:O	2.06	0.88
1:E:165:GLN:H	1:E:165:GLN:HE21	1.21	0.88
1:D:165:GLN:H	1:D:165:GLN:HE21	1.16	0.88
1:F:165:GLN:H	1:F:165:GLN:HE21	1.18	0.88
1:B:64:ARG:NH1	1:B:100:ASP:O	2.07	0.86
2:M:390:LYS:HD2	6:M:641:HOH:O	1.74	0.86
2:Q:361:HIS:CD2	2:Q:361:HIS:H	1.91	0.86
1:E:64:ARG:NH1	1:E:100:ASP:O	2.08	0.85
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.57	0.85
1:D:78:GLU:HG2	2:P:301:PRO:HG2	1.58	0.84
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.60	0.83
2:Q:390:LYS:HD3	6:Q:1020:HOH:O	1.77	0.83
1:F:176:GLU:HG3	1:F:180:LYS:O	1.79	0.83
2:R:497:ASN:ND2	2:R:499:GLU:H	1.75	0.83
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.60	0.81
1:A:165:GLN:H	1:A:165:GLN:NE2	1.79	0.81
2:N:488:MET:CE	1:C:1:PRO:HG3	2.10	0.80
2:R:361:HIS:H	2:R:361:HIS:CD2	1.98	0.78
1:C:165:GLN:H	1:C:165:GLN:NE2	1.81	0.78
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.66	0.77
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.32	0.77
2:M:361:HIS:H	2:M:361:HIS:CD2	2.02	0.77
1:C:165:GLN:H	1:C:165:GLN:HE21	1.29	0.77
1:E:165:GLN:H	1:E:165:GLN:NE2	1.83	0.77
2:P:361:HIS:H	2:P:361:HIS:CD2	1.99	0.76
2:N:497:ASN:ND2	2:N:499:GLU:H	1.83	0.76
1:B:176:GLU:HG3	1:B:180:LYS:O	1.85	0.76
1:D:165:GLN:H	1:D:165:GLN:NE2	1.82	0.76
2:R:306:SER:CB	2:R:530:GLN:HE21	1.98	0.76
2:O:497:ASN:HD22	2:O:499:GLU:H	1.34	0.75
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.68	0.75
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.68	0.75
2:N:497:ASN:HD22	2:N:499:GLU:H	1.32	0.75
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.67	0.75
2:N:453:PRO:HB2	2:O:310:ILE:HD12	1.70	0.74
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.32	0.74
2:M:497:ASN:HD22	2:M:499:GLU:H	1.32	0.73
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.20	0.73
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.71	0.73
2:R:361:HIS:H	2:R:361:HIS:HD2	1.37	0.73
2:P:361:HIS:H	2:P:361:HIS:HD2	1.37	0.72
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.72
2:O:497:ASN:ND2	2:O:499:GLU:H	1.86	0.72
1:B:165:GLN:H	1:B:165:GLN:HE21	0.76	0.72
1:D:78:GLU:CG	2:P:301:PRO:HG2	2.21	0.71
1:D:176:GLU:HG3	1:D:180:LYS:O	1.90	0.71
2:M:361:HIS:H	2:M:361:HIS:HD2	1.39	0.70
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.57	0.70
1:F:3:GLU:OE1	1:F:3:GLU:HA	1.92	0.69
1:A:176:GLU:HG3	1:A:180:LYS:O	1.93	0.69
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.57	0.69
1:B:103:GLU:OE2	1:B:184:ARG:NH2	2.23	0.69
2:R:416:LEU:C	2:R:416:LEU:HD23	2.18	0.69
2:M:416:LEU:C	2:M:416:LEU:HD23	2.17	0.69
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:536:GLU:HB2	6:R:1336:HOH:O	1.93	0.68
2:N:361:HIS:CD2	2:N:361:HIS:H	2.11	0.68
1:E:100:ASP:OD1	1:E:100:ASP:N	2.26	0.68
2:Q:522:ARG:NH1	6:Q:1057:HOH:O	2.26	0.67
2:M:536:GLU:HB2	6:M:698:HOH:O	1.95	0.67
2:P:497:ASN:HD22	2:P:499:GLU:H	1.41	0.67
2:Q:399:MET:HA	2:Q:462:HIS:O	1.96	0.66
2:M:497:ASN:ND2	2:M:499:GLU:H	1.93	0.66
2:Q:356:PHE:CZ	2:Q:430:LEU:HD13	2.30	0.66
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.28	0.66
1:D:65:ASP:OD2	1:D:133:ARG:HD3	1.96	0.66
2:O:361:HIS:H	2:O:361:HIS:CD2	2.14	0.65
1:D:100:ASP:OD1	1:D:100:ASP:N	2.28	0.65
2:P:416:LEU:C	2:P:416:LEU:HD23	2.22	0.65
2:O:390:LYS:HE2	6:O:727:HOH:O	1.96	0.65
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.60	0.65
1:D:79:TYR:O	2:P:301:PRO:HB3	1.96	0.65
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.21	0.65
2:O:478:LEU:HD23	2:O:478:LEU:C	2.21	0.64
1:C:19:ILE:O	2:O:426:VAL:HG21	1.98	0.64
2:Q:390:LYS:HE2	6:Q:1137:HOH:O	1.97	0.64
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.33	0.64
1:A:79:TYR:O	2:M:301:PRO:HB2	1.98	0.63
2:M:522:ARG:NH1	6:M:665:HOH:O	2.28	0.63
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.81	0.63
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.79	0.63
2:R:497:ASN:HD22	2:R:499:GLU:N	1.93	0.63
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.27	0.63
2:P:497:ASN:ND2	2:P:499:GLU:H	1.96	0.62
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.65	0.62
1:F:48:HIS:HA	1:F:109:VAL:HG12	1.82	0.62
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.00	0.62
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.34	0.62
2:R:497:ASN:HD22	2:R:497:ASN:C	2.08	0.62
2:M:359:HIS:O	2:M:366:ASN:HB3	2.00	0.62
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.35	0.62
1:F:70:VAL:HG21	1:F:106:LEU:HD21	1.81	0.61
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.65	0.61
2:N:488:MET:HE1	1:C:1:PRO:HG3	1.81	0.61
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.83	0.61
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.34	0.61
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.83	0.61
2:N:400:TRP:HA	2:N:425:GLY:O	2.00	0.61
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.98	0.61
1:F:143:LEU:C	1:F:143:LEU:HD23	2.26	0.61
2:Q:364:LEU:HD11	2:Q:442:ILE:HG23	1.81	0.61
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.26	0.61
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.83	0.60
2:N:359:HIS:O	2:N:366:ASN:HB3	2.01	0.60
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.81	0.60
2:Q:473:LYS:NZ	6:Q:1036:HOH:O	2.31	0.60
1:F:25:ALA:O	2:R:411:LYS:NZ	2.34	0.60
1:F:176:GLU:HG3	1:F:180:LYS:C	2.26	0.60
1:F:19:ILE:O	2:R:426:VAL:HG21	2.01	0.60
1:F:131:PHE:O	1:F:132:ALA:HB2	2.02	0.60
2:P:405:GLY:HA3	6:P:651:HOH:O	2.02	0.59
1:B:176:GLU:OE2	1:B:179:GLY:O	2.20	0.59
1:F:50:LEU:O	1:F:182:ALA:HA	2.01	0.59
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.65	0.59
1:E:24:GLU:O	1:E:27:GLY:N	2.35	0.59
2:N:399:MET:HA	2:N:462:HIS:O	2.01	0.59
1:A:78:GLU:HG2	2:M:301:PRO:HG3	1.84	0.59
1:E:143:LEU:HD23	1:E:143:LEU:C	2.28	0.58
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.68	0.58
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.85	0.58
1:D:78:GLU:CD	2:P:301:PRO:HG2	2.28	0.58
1:D:143:LEU:C	1:D:143:LEU:HD23	2.28	0.58
1:C:79:TYR:O	2:O:301:PRO:HB3	2.03	0.58
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.03	0.58
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.84	0.58
1:C:15:PRO:HD2	3:O:575:CYN:N	2.17	0.58
2:O:359:HIS:O	2:O:366:ASN:HB3	2.03	0.58
1:D:131:PHE:O	1:D:132:ALA:HB2	2.03	0.58
2:R:406:GLY:O	2:R:447:TYR:HD1	1.87	0.58
2:O:416:LEU:C	2:O:416:LEU:HD23	2.27	0.58
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.03	0.58
2:N:497:ASN:HD22	2:N:497:ASN:C	2.10	0.58
2:P:390:LYS:HD2	6:P:648:HOH:O	2.05	0.57
2:N:364:LEU:HD12	2:N:373:PRO:HG2	1.86	0.57
1:E:176:GLU:HG3	1:E:180:LYS:O	2.04	0.57
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:416:LEU:C	2:M:416:LEU:CD2	2.77	0.57
2:P:400:TRP:HA	2:P:425:GLY:O	2.04	0.57
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.04	0.57
1:A:165:GLN:H	1:A:165:GLN:CD	2.13	0.56
1:B:70:VAL:HG21	1:B:106:LEU:HD21	1.85	0.56
1:B:147:ASP:OD2	1:B:174:ARG:NH1	2.38	0.56
1:F:115:ASN:HA	1:F:121:PRO:HA	1.86	0.56
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.87	0.56
1:B:176:GLU:HG3	1:B:180:LYS:C	2.30	0.56
2:R:536:GLU:HG3	6:R:1229:HOH:O	2.04	0.56
1:D:77:GLY:O	1:D:114:VAL:HG12	2.05	0.56
2:R:416:LEU:HD23	2:R:417:ALA:N	2.19	0.56
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.35	0.56
2:N:361:HIS:H	2:N:361:HIS:HD2	1.54	0.56
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.56
1:A:176:GLU:HA	1:A:180:LYS:O	2.05	0.56
3:M:575:CYN:N	6:M:602:HOH:O	2.33	0.56
2:P:376:GLU:O	2:P:442:ILE:HA	2.05	0.56
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.39	0.56
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.42	0.55
1:F:74:ASP:OD1	1:F:74:ASP:C	2.47	0.55
2:Q:364:LEU:CD2	2:Q:440:ARG:HD3	2.36	0.55
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.54	0.55
1:B:165:GLN:NE2	1:B:165:GLN:N	2.34	0.55
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.02	0.55
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.88	0.55
1:F:35:ILE:HD13	2:R:351:PHE:CE1	2.41	0.55
1:F:37:ASN:HB2	1:F:106:LEU:HD12	1.87	0.55
1:D:98:THR:O	1:D:102:GLY:HA2	2.07	0.55
1:C:100:ASP:OD1	1:C:100:ASP:N	2.39	0.54
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.07	0.54
2:O:326:THR:HG22	2:O:326:THR:O	2.06	0.54
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.05	0.54
2:Q:356:PHE:HD1	2:Q:428:ARG:HD2	1.72	0.54
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.05	0.54
1:E:98:THR:O	1:E:102:GLY:HA2	2.08	0.54
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.55	0.54
2:M:406:GLY:O	2:M:447:TYR:HD1	1.91	0.54
2:N:383:ARG:NE	2:N:434:ASP:O	2.40	0.54
2:Q:356:PHE:HZ	2:Q:430:LEU:HD13	1.73	0.54
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:497:ASN:HD22	2:O:497:ASN:C	2.16	0.54
2:O:522:ARG:NH1	6:O:673:HOH:O	2.36	0.54
1:F:15:PRO:HD2	3:R:575:CYN:N	2.22	0.54
2:O:406:GLY:O	2:O:447:TYR:HD1	1.90	0.54
1:D:165:GLN:HE21	1:D:165:GLN:N	1.97	0.54
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.54
2:Q:487:PRO:O	2:Q:493:LYS:HD3	2.08	0.53
1:F:165:GLN:HE21	1:F:165:GLN:N	1.97	0.53
1:F:174:ARG:HB2	1:F:183:TYR:CE1	2.43	0.53
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.90	0.53
2:O:376:GLU:O	2:O:442:ILE:HA	2.08	0.53
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.90	0.53
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.43	0.53
1:C:36:TRP:CG	1:C:37:ASN:H	2.27	0.53
2:O:356:PHE:HE1	2:O:428:ARG:HD3	1.74	0.53
1:D:134:GLY:CA	2:P:326:THR:HG22	2.37	0.53
2:N:488:MET:HE2	1:C:1:PRO:HG3	1.91	0.53
2:M:405:GLY:HA3	6:M:644:HOH:O	2.07	0.53
1:B:98:THR:O	1:B:102:GLY:HA2	2.08	0.53
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.90	0.53
2:R:405:GLY:HA3	6:R:1260:HOH:O	2.09	0.53
2:R:306:SER:HB3	2:R:530:GLN:HE21	1.73	0.53
2:R:359:HIS:O	2:R:366:ASN:HB3	2.08	0.53
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.08	0.53
2:P:497:ASN:HD22	2:P:497:ASN:C	2.17	0.53
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.45	0.53
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.09	0.53
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.24	0.52
2:N:363:LEU:HD11	2:N:427:GLY:HA3	1.91	0.52
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.92	0.52
1:D:1:PRO:HG2	2:R:488:MET:HE2	1.92	0.52
1:E:15:PRO:HD2	3:Q:575:CYN:N	2.25	0.52
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.44	0.52
1:B:16:TYR:OH	2:N:447:TYR:OH	2.26	0.52
2:O:306:SER:CB	2:O:530:GLN:HE21	2.23	0.52
2:P:390:LYS:NZ	6:P:666:HOH:O	2.43	0.52
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.73	0.52
2:M:399:MET:HA	2:M:462:HIS:O	2.10	0.51
2:O:385:VAL:HA	2:O:390:LYS:O	2.10	0.51
2:Q:483:ASP:HB3	2:Q:486:ILE:HG13	1.91	0.51
1:D:33:GLN:HB3	1:D:85:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.92	0.51
2:O:306:SER:OG	2:O:530:GLN:NE2	2.37	0.51
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.93	0.51
1:D:15:PRO:HD2	3:P:575:CYN:N	2.26	0.51
2:M:400:TRP:HA	2:M:425:GLY:O	2.11	0.51
1:C:38:ARG:HG3	1:C:107:HIS:HB2	1.92	0.51
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.24	0.51
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.92	0.51
2:P:416:LEU:C	2:P:416:LEU:CD2	2.84	0.51
2:P:536:GLU:HB2	6:P:702:HOH:O	2.11	0.51
1:E:98:THR:HB	1:E:100:ASP:OD1	2.11	0.51
1:D:33:GLN:HB3	1:D:85:LEU:HD11	1.92	0.51
2:N:497:ASN:HD22	2:N:498:PRO:N	2.10	0.50
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.38	0.50
1:E:33:GLN:O	2:Q:428:ARG:NH2	2.41	0.50
1:E:36:TRP:CG	1:E:37:ASN:H	2.28	0.50
1:A:188:ARG:NH1	6:A:259:HOH:O	2.43	0.50
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.92	0.50
1:D:32:ASP:HB2	6:P:730:HOH:O	2.10	0.50
1:E:32:ASP:HB2	6:E:267:HOH:O	2.10	0.50
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.93	0.50
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.66	0.50
1:B:36:TRP:CG	1:B:37:ASN:H	2.28	0.50
1:D:19:ILE:O	2:P:426:VAL:HG21	2.10	0.50
1:C:176:GLU:HA	1:C:180:LYS:O	2.11	0.50
2:N:478:LEU:C	2:N:478:LEU:HD23	2.36	0.50
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.92	0.50
1:A:157:VAL:O	1:A:160:LEU:HB2	2.11	0.50
1:B:143:LEU:C	1:B:143:LEU:HD23	2.37	0.50
1:C:74:ASP:C	1:C:74:ASP:OD1	2.55	0.50
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.93	0.50
2:R:399:MET:HA	2:R:462:HIS:O	2.12	0.50
1:A:78:GLU:CG	2:M:301:PRO:HG3	2.42	0.50
1:B:64:ARG:HD3	1:B:99:PHE:O	2.12	0.50
2:O:356:PHE:CD1	2:O:428:ARG:HD2	2.46	0.50
1:F:31:ARG:HH11	2:R:428:ARG:HG2	1.75	0.50
2:M:478:LEU:HD23	2:M:478:LEU:C	2.37	0.50
2:P:302:ALA:HB1	2:P:347:THR:HG22	1.93	0.50
2:P:478:LEU:C	2:P:478:LEU:HD23	2.37	0.50
2:M:497:ASN:HD22	2:M:499:GLU:N	2.07	0.49
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.12	0.49
2:N:536:GLU:HB2	6:N:701:HOH:O	2.12	0.49
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.39	0.49
1:D:176:GLU:HG3	1:D:180:LYS:C	2.37	0.49
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.95	0.49
1:A:92:PHE:CG	2:M:349:PRO:HG3	2.47	0.49
1:B:134:GLY:HA3	2:N:326:THR:HG22	1.94	0.49
2:O:497:ASN:HD22	2:O:498:PRO:N	2.09	0.49
2:N:406:GLY:O	2:N:447:TYR:HD1	1.94	0.49
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.76	0.49
2:P:522:ARG:NH1	6:P:670:HOH:O	2.37	0.49
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.43	0.49
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.95	0.49
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.28	0.49
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.28	0.49
1:E:176:GLU:HG3	1:E:180:LYS:C	2.38	0.49
2:Q:356:PHE:CD1	2:Q:428:ARG:HD2	2.48	0.49
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.20	0.49
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.76	0.49
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.48	0.49
1:E:165:GLN:HE21	1:E:165:GLN:N	2.01	0.49
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.13	0.48
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.28	0.48
1:E:10:SER:O	1:E:11:GLN:HG2	2.13	0.48
2:R:390:LYS:HE2	6:R:1373:HOH:O	2.13	0.48
1:A:98:THR:O	1:A:102:GLY:HA2	2.14	0.48
2:M:361:HIS:CD2	2:M:361:HIS:N	2.73	0.48
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.47	0.48
1:C:176:GLU:HG3	1:C:180:LYS:C	2.38	0.48
2:P:488:MET:C	2:P:493:LYS:HE2	2.38	0.48
1:E:52:LEU:HD23	1:E:184:ARG:NH1	2.28	0.48
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.49	0.48
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.13	0.48
2:O:356:PHE:CD1	2:O:428:ARG:CD	2.96	0.48
1:D:33:GLN:CD	1:D:85:LEU:HD12	2.39	0.48
1:F:35:ILE:CD1	2:R:351:PHE:CE1	2.96	0.48
1:D:98:THR:OG1	1:D:102:GLY:N	2.38	0.48
1:B:3:GLU:CA	1:B:3:GLU:OE1	2.61	0.48
1:B:132:ALA:HB3	1:B:135:ILE:HD12	1.96	0.48
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.94	0.48
1:F:77:GLY:O	1:F:114:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.96	0.48
2:N:356:PHE:CZ	2:N:430:LEU:HD13	2.49	0.48
1:F:64:ARG:HD3	1:F:99:PHE:O	2.14	0.48
1:D:36:TRP:CG	1:D:37:ASN:H	2.32	0.48
1:D:39:LEU:HD12	1:D:39:LEU:N	2.29	0.48
1:D:191:GLY:O	1:D:194:GLU:HB2	2.14	0.48
2:R:497:ASN:ND2	2:R:499:GLU:N	2.54	0.48
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.14	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.48	0.48
1:C:131:PHE:O	1:C:132:ALA:HB2	2.14	0.47
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.79	0.47
1:A:100:ASP:OD1	1:A:100:ASP:N	2.44	0.47
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.96	0.47
2:O:302:ALA:HB1	2:O:347:THR:CG2	2.44	0.47
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.96	0.47
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.96	0.47
1:D:26:ALA:O	2:P:411:LYS:HG3	2.14	0.47
2:P:359:HIS:O	2:P:366:ASN:HB3	2.13	0.47
2:P:399:MET:HA	2:P:462:HIS:O	2.14	0.47
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.14	0.47
1:A:36:TRP:CG	1:A:37:ASN:H	2.33	0.47
1:D:15:PRO:HB3	1:D:133:ARG:HD2	1.96	0.47
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.49	0.47
1:D:50:LEU:O	1:D:182:ALA:HA	2.14	0.47
1:D:51:LEU:O	1:D:105:THR:HA	2.14	0.47
1:E:51:LEU:HD11	1:E:126:ILE:HD12	1.96	0.47
2:Q:415:TYR:CE1	2:Q:416:LEU:HD23	2.49	0.47
1:F:98:THR:O	1:F:102:GLY:HA2	2.15	0.47
2:R:306:SER:OG	2:R:530:GLN:NE2	2.48	0.47
2:R:394:ASN:HA	2:R:431:THR:O	2.15	0.47
1:A:180:LYS:HG2	1:A:181:THR:N	2.29	0.47
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.15	0.47
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.30	0.47
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.96	0.47
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.84	0.47
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.80	0.47
2:R:400:TRP:HA	2:R:425:GLY:O	2.15	0.47
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.97	0.47
1:A:6:PRO:HG2	2:M:503:GLN:NE2	2.31	0.47
2:M:363:LEU:N	2:M:363:LEU:HD12	2.30	0.47
2:M:392:VAL:HG12	2:M:395:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.74	0.47
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.97	0.47
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.14	0.47
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.96	0.46
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.50	0.46
2:Q:304:ASP:OD1	2:Q:307:ARG:NH1	2.37	0.46
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.83	0.46
2:N:486:ILE:N	2:N:487:PRO:HD2	2.30	0.46
2:Q:536:GLU:HB2	6:Q:1100:HOH:O	2.15	0.46
1:F:143:LEU:HD23	1:F:144:TYR:N	2.30	0.46
1:E:19:ILE:O	2:Q:426:VAL:CG2	2.64	0.46
1:E:131:PHE:O	1:E:132:ALA:HB2	2.16	0.46
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.15	0.46
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.50	0.46
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.62	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.31	0.46
1:D:92:PHE:CG	2:P:349:PRO:HG3	2.51	0.46
1:F:165:GLN:NE2	1:F:165:GLN:N	2.49	0.46
1:C:113:VAL:HG13	1:C:122:MET:O	2.15	0.46
2:O:313:ARG:O	2:O:318:LYS:HE2	2.16	0.46
1:E:147:ASP:OD2	1:E:174:ARG:NH1	2.48	0.46
2:R:356:PHE:CE1	2:R:428:ARG:HD3	2.51	0.46
1:A:155:CYS:O	1:A:159:ASN:ND2	2.49	0.46
1:B:1:PRO:HA	2:P:508:LEU:O	2.16	0.46
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.75	0.46
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.84	0.46
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.67	0.46
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.30	0.46
2:M:512:ASN:O	2:Q:534:HIS:HE1	1.99	0.46
1:B:50:LEU:O	1:B:182:ALA:HA	2.16	0.46
1:E:51:LEU:HB2	1:E:106:LEU:HB3	1.98	0.46
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.64	0.46
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.16	0.46
2:N:486:ILE:HB	2:N:487:PRO:HD3	1.97	0.46
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.85	0.46
2:Q:362:ASP:OD2	2:Q:440:ARG:NH1	2.48	0.46
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.98	0.45
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.85	0.45
1:C:98:THR:OG1	1:C:102:GLY:N	2.50	0.45
2:O:318:LYS:HA	2:O:318:LYS:HD3	1.64	0.45
2:O:364:LEU:CD2	2:O:440:ARG:HD3	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:376:GLU:OE1	6:P:642:HOH:O	2.21	0.45
2:Q:356:PHE:HE2	2:Q:430:LEU:HD22	1.81	0.45
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.38	0.45
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.52	0.45
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.98	0.45
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.97	0.45
1:F:41:LYS:O	1:F:44:ALA:N	2.49	0.45
2:M:390:LYS:HD3	6:M:717:HOH:O	2.16	0.45
1:C:98:THR:O	1:C:102:GLY:HA2	2.17	0.45
1:E:56:TYR:CE2	1:E:62:LEU:HD23	2.52	0.45
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.17	0.45
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.44	0.45
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.80	0.45
2:O:400:TRP:HA	2:O:425:GLY:O	2.15	0.45
1:F:32:ASP:HB2	6:R:1383:HOH:O	2.17	0.45
2:P:483:ASP:HB3	2:P:486:ILE:HG13	1.99	0.45
1:F:74:ASP:OD1	1:F:76:ASN:N	2.50	0.45
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.69	0.45
1:F:58:GLY:HA3	1:F:190:GLN:OE1	2.16	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.42	0.45
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.47	0.45
2:M:326:THR:HG22	2:M:326:THR:O	2.17	0.45
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.52	0.45
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.45
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.99	0.45
2:P:360:ASP:O	2:P:427:GLY:HA2	2.17	0.45
1:B:98:THR:HB	1:B:100:ASP:OD1	2.17	0.44
1:B:114:VAL:HG22	1:B:122:MET:HE3	1.98	0.44
2:R:378:ILE:HA	2:R:519:LEU:O	2.17	0.44
1:E:176:GLU:HA	1:E:180:LYS:O	2.17	0.44
2:N:386:ASP:HA	2:N:527:LEU:O	2.18	0.44
1:C:143:LEU:HD23	1:C:143:LEU:C	2.42	0.44
1:F:98:THR:OG1	1:F:101:ALA:HB3	2.17	0.44
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.52	0.44
1:C:16:TYR:O	1:C:19:ILE:HG23	2.18	0.44
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.98	0.44
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.99	0.44
2:Q:428:ARG:O	2:Q:429:CYS:HB3	2.17	0.44
1:F:39:LEU:N	1:F:39:LEU:HD12	2.33	0.44
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.65	0.44
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:395:THR:O	2:Q:430:LEU:HA	2.18	0.44
2:N:364:LEU:HD11	2:N:442:ILE:HG23	2.00	0.44
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	1.99	0.44
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.89	0.44
2:R:307:ARG:CG	2:R:533:THR:HG22	2.48	0.44
2:R:326:THR:HG22	2:R:330:ARG:HD2	2.00	0.44
1:A:50:LEU:O	1:A:182:ALA:HA	2.17	0.44
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.98	0.44
1:E:134:GLY:HA3	2:Q:326:THR:HG22	2.00	0.44
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.17	0.44
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.46	0.44
2:M:497:ASN:HD22	2:M:497:ASN:C	2.26	0.44
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.52	0.44
1:A:1:PRO:HG2	2:O:488:MET:HE2	1.99	0.43
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.53	0.43
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.89	0.43
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.48	0.43
1:A:24:GLU:O	1:A:27:GLY:N	2.47	0.43
2:R:416:LEU:C	2:R:416:LEU:CD2	2.90	0.43
2:N:395:THR:O	2:N:430:LEU:HA	2.18	0.43
1:D:5:LEU:O	2:P:387:GLN:HG2	2.19	0.43
2:Q:363:LEU:HD11	2:Q:427:GLY:HA3	1.99	0.43
2:O:361:HIS:H	2:O:361:HIS:HD2	1.61	0.43
1:E:1:PRO:HB2	6:E:201:HOH:O	2.17	0.43
2:Q:366:ASN:OD1	2:Q:366:ASN:C	2.62	0.43
1:A:15:PRO:HB3	1:A:133:ARG:HD2	2.00	0.43
2:R:383:ARG:HA	2:R:435:GLY:O	2.19	0.43
1:B:66:SER:HB2	1:B:130:LEU:HD11	2.01	0.43
2:P:495:ILE:CG2	2:P:500:ALA:HB3	2.49	0.43
1:E:94:ARG:HH11	1:E:94:ARG:HD3	1.71	0.43
1:A:64:ARG:HD3	1:A:99:PHE:O	2.19	0.43
1:E:18:HIS:CE1	1:E:99:PHE:CE1	3.06	0.43
2:R:311:ARG:HH11	2:R:311:ARG:HD2	1.67	0.43
2:M:362:ASP:OD2	2:M:440:ARG:NH1	2.52	0.43
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.73	0.43
1:C:18:HIS:CE1	1:C:99:PHE:CE1	3.07	0.43
2:O:360:ASP:HB3	2:O:428:ARG:HG3	2.01	0.43
2:R:432:ASP:OD1	2:R:432:ASP:C	2.62	0.43
1:B:5:LEU:O	2:N:387:GLN:HG2	2.19	0.43
1:D:39:LEU:HB3	1:D:90:ASN:O	2.19	0.43
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:NE2	1:A:165:GLN:N	2.59	0.42
2:N:497:ASN:ND2	2:N:499:GLU:OE1	2.43	0.42
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.31	0.42
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.39	0.42
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.38	0.42
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.83	0.42
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.34	0.42
2:N:307:ARG:HA	2:N:307:ARG:HD3	1.79	0.42
1:E:52:LEU:C	1:E:52:LEU:HD22	2.44	0.42
2:N:486:ILE:N	2:N:487:PRO:CD	2.82	0.42
2:O:483:ASP:HA	2:O:484:PRO:HD2	1.94	0.42
1:D:176:GLU:HG2	1:D:179:GLY:CA	2.49	0.42
1:F:36:TRP:CG	1:F:37:ASN:H	2.37	0.42
2:M:483:ASP:HB3	2:M:486:ILE:HG13	2.02	0.42
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.01	0.42
2:N:356:PHE:HZ	2:N:430:LEU:HD13	1.85	0.42
1:E:110:LYS:CE	1:E:148:GLU:OE2	2.67	0.42
1:F:8:THR:HA	1:F:9:PRO:HD3	1.87	0.42
2:R:447:TYR:HA	2:R:448:PRO:HD3	1.89	0.42
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.41	0.42
1:A:36:TRP:CE3	1:A:36:TRP:HA	2.54	0.42
2:N:516:MET:HE3	2:N:516:MET:HB3	1.83	0.42
2:P:489:CYS:C	2:P:493:LYS:HE3	2.44	0.42
2:N:522:ARG:HD3	6:N:669:HOH:O	2.19	0.42
2:O:437:TYR:CD1	2:O:437:TYR:C	2.97	0.42
2:Q:362:ASP:OD1	2:Q:364:LEU:HB2	2.20	0.42
2:R:442:ILE:O	2:R:442:ILE:HG13	2.19	0.42
2:M:448:PRO:HB2	2:P:516:MET:HA	2.01	0.42
2:P:302:ALA:HB1	2:P:347:THR:CG2	2.50	0.42
1:C:38:ARG:HH11	1:C:38:ARG:HD2	1.68	0.42
1:C:155:CYS:HB3	1:C:158:LEU:HB2	2.02	0.42
1:D:23:LEU:O	1:D:24:GLU:C	2.63	0.42
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.20	0.42
2:M:307:ARG:HD2	6:M:653:HOH:O	2.18	0.41
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.19	0.41
2:P:363:LEU:HD11	2:P:427:GLY:HA3	2.00	0.41
2:N:386:ASP:C	2:N:386:ASP:OD1	2.63	0.41
1:D:131:PHE:O	1:D:132:ALA:CB	2.68	0.41
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.20	0.41
1:E:161:ILE:O	1:E:167:ARG:NH2	2.48	0.41
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:420:ASP:HA	2:M:421:PRO:HD2	1.89	0.41
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.20	0.41
1:E:124:PRO:HA	6:E:221:HOH:O	2.19	0.41
2:R:497:ASN:ND2	2:R:497:ASN:C	2.76	0.41
1:A:143:LEU:C	1:A:143:LEU:HD23	2.45	0.41
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.85	0.41
2:M:324:TYR:OH	5:M:550:NNO:O1	2.31	0.41
2:M:371:GLY:HA3	2:M:422:ASN:ND2	2.36	0.41
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.92	0.41
2:N:416:LEU:HD23	2:N:416:LEU:C	2.45	0.41
1:D:18:HIS:NE2	6:D:944:HOH:O	2.27	0.41
1:D:72:GLN:O	1:D:91:SER:OG	2.34	0.41
2:M:376:GLU:O	2:M:442:ILE:HA	2.21	0.41
2:P:497:ASN:HD22	2:P:498:PRO:N	2.18	0.41
1:F:44:ALA:O	1:F:48:HIS:NE2	2.36	0.41
2:R:376:GLU:O	2:R:442:ILE:HA	2.21	0.41
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.55	0.41
2:M:302:ALA:HB1	2:M:347:THR:CG2	2.50	0.41
2:M:437:TYR:CD1	2:M:437:TYR:C	2.98	0.41
2:M:484:PRO:O	2:M:487:PRO:HD2	2.21	0.41
2:N:453:PRO:CB	2:O:310:ILE:HD12	2.46	0.41
1:C:19:ILE:HG13	2:O:426:VAL:HG22	2.02	0.41
1:B:6:PRO:HG2	2:N:503:GLN:NE2	2.35	0.41
2:O:390:LYS:HD3	6:O:651:HOH:O	2.20	0.41
1:E:123:ALA:O	1:E:124:PRO:C	2.63	0.41
2:Q:415:TYR:CE1	2:Q:416:LEU:CD2	3.04	0.41
1:F:78:GLU:HB2	1:F:80:GLN:NE2	2.36	0.41
2:R:516:MET:HE3	2:R:516:MET:HB3	1.82	0.41
2:P:392:VAL:HG12	2:P:395:THR:HB	2.01	0.41
1:E:35:ILE:HG22	1:E:94:ARG:HG3	2.02	0.41
1:F:19:ILE:O	2:R:426:VAL:CG2	2.68	0.41
1:A:35:ILE:CD1	2:M:351:PHE:CE1	3.04	0.41
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.36	0.41
1:E:110:LYS:HE2	1:E:148:GLU:OE2	2.21	0.41
2:Q:406:GLY:O	2:Q:447:TYR:HD1	2.04	0.41
2:N:318:LYS:HA	2:N:318:LYS:HD3	1.80	0.41
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.21	0.41
2:P:383:ARG:NE	2:P:434:ASP:O	2.41	0.41
2:O:405:GLY:HA3	6:O:654:HOH:O	2.20	0.40
2:P:534:HIS:O	2:P:535:PHE:C	2.64	0.40
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:495:ILE:HG21	2:R:500:ALA:HB3	2.04	0.40
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.51	0.40
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.22	0.40
1:B:79:TYR:O	2:N:301:PRO:CB	2.70	0.40
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.63	0.40
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.18	0.40
2:Q:513:ALA:O	2:Q:515:PRO:HD3	2.21	0.40
1:F:44:ALA:HA	1:F:45:PRO:HD2	1.82	0.40
2:R:316:HIS:HB3	2:R:317:PRO:HD2	2.04	0.40
2:N:493:LYS:HB2	2:N:493:LYS:HE3	1.69	0.40
2:O:478:LEU:C	2:O:478:LEU:CD2	2.93	0.40
2:M:360:ASP:O	2:M:427:GLY:HA2	2.21	0.40
1:C:19:ILE:HD13	1:C:19:ILE:HG21	1.74	0.40
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.57	0.40
1:D:64:ARG:HD3	1:D:99:PHE:O	2.21	0.40
2:P:516:MET:HE3	2:P:516:MET:HB3	1.93	0.40
1:E:39:LEU:HD11	1:E:93:GLY:HA3	2.02	0.40
2:Q:310:ILE:HD13	2:Q:310:ILE:HA	1.82	0.40
1:A:70:VAL:HA	1:A:127:ASN:O	2.21	0.40
1:B:114:VAL:CG2	1:B:122:MET:HE3	2.52	0.40
2:O:378:ILE:HA	2:O:519:LEU:O	2.21	0.40
1:D:52:LEU:HA	1:D:104:TRP:O	2.21	0.40
2:P:328:ILE:HD12	2:Q:335:ALA:HB2	2.02	0.40
2:R:465:ILE:HD12	2:R:465:ILE:N	2.36	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	178/200 (89%)	169 (95%)	9 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	D	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	24	24
1	E	198/200 (99%)	186 (94%)	12 (6%)	0	100	100
1	F	198/200 (99%)	187 (94%)	9 (4%)	2 (1%)	12	10
2	M	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	N	229/238 (96%)	219 (96%)	9 (4%)	1 (0%)	30	31
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	31
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	31
All	All	2542/2628 (97%)	2431 (96%)	105 (4%)	6 (0%)	43	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	535	PHE
2	R	535	PHE
2	N	535	PHE
1	D	132	ALA
1	F	132	ALA
1	F	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	153 (94%)	9 (6%)	19	20
1	B	162/163 (99%)	155 (96%)	7 (4%)	26	31
1	C	162/163 (99%)	155 (96%)	7 (4%)	26	31
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	37
1	F	162/163 (99%)	156 (96%)	6 (4%)	30	37
2	M	196/202 (97%)	187 (95%)	9 (5%)	24	28
2	N	196/202 (97%)	191 (97%)	5 (3%)	40	50
2	O	196/202 (97%)	186 (95%)	10 (5%)	21	23
2	P	196/202 (97%)	186 (95%)	10 (5%)	21	23
2	Q	196/202 (97%)	184 (94%)	12 (6%)	17	17
2	R	196/202 (97%)	187 (95%)	9 (5%)	24	28
All	All	2148/2190 (98%)	2050 (95%)	98 (5%)	24	28

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	24	GLU
1	A	38	ARG
1	A	52	LEU
1	A	78	GLU
1	A	94	ARG
1	A	114	VAL
1	A	165	GLN
2	M	301	PRO
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	429	CYS
2	M	488	MET
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	24	GLU
1	B	32	ASP
1	B	52	LEU
1	B	114	VAL
1	B	165	GLN
1	B	176	GLU
2	N	364	LEU

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Mol	Chain	Res	Type
2	N	395	THR
2	N	416	LEU
2	N	497	ASN
2	N	499	GLU
1	C	4	LEU
1	C	19	ILE
1	C	24	GLU
1	C	52	LEU
1	C	66	SER
1	C	100	ASP
1	C	165	GLN
2	O	364	LEU
2	O	372	LEU
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	429	CYS
2	O	434	ASP
2	O	478	LEU
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	43	ASP
1	D	52	LEU
1	D	100	ASP
1	D	114	VAL
1	D	165	GLN
2	P	364	LEU
2	P	395	THR
2	P	416	LEU
2	P	428	ARG
2	P	433	SER
2	P	434	ASP
2	P	478	LEU
2	P	507	LYS
2	P	511	ASN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	52	LEU

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Mol	Chain	Res	Type
1	E	100	ASP
1	E	114	VAL
1	E	165	GLN
2	Q	364	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	429	CYS
2	Q	434	ASP
2	Q	438	SER
2	Q	478	LEU
2	Q	493	LYS
2	Q	497	ASN
2	Q	507	LYS
2	Q	515	PRO
1	F	4	LEU
1	F	19	ILE
1	F	24	GLU
1	F	52	LEU
1	F	94	ARG
1	F	165	GLN
2	R	306	SER
2	R	343	ILE
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	433	SER
2	R	434	ASP
2	R	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	165	GLN
2	M	361	HIS
2	M	422	ASN
2	M	497	ASN
2	M	503	GLN
1	B	37	ASN
1	B	140	HIS

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	165	GLN
2	N	334	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	163	GLN
1	C	165	GLN
2	O	305	ASN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	59	ASN
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	502	GLN
2	P	503	GLN
2	P	530	GLN
1	E	163	GLN
1	E	165	GLN
2	Q	334	GLN
2	Q	361	HIS
2	Q	422	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
2	Q	534	HIS
1	F	11	GLN
1	F	18	HIS
1	F	127	ASN
1	F	163	GLN
1	F	165	GLN
2	R	361	HIS
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYN	P	575	4	1,1,1	0.52	0	-		
3	CYN	Q	575	4	1,1,1	0.50	0	-		
5	NNO	O	550	4	11,11,11	2.17	3 (27%)	11,15,15	1.67	2 (18%)
5	NNO	R	550	4	11,11,11	1.93	3 (27%)	11,15,15	1.49	2 (18%)
5	NNO	Q	550	4	11,11,11	2.04	2 (18%)	11,15,15	1.23	1 (9%)
3	CYN	M	575	4	1,1,1	0.62	0	-		
3	CYN	N	575	4	1,1,1	0.53	0	-		
3	CYN	R	575	4	1,1,1	0.55	0	-		
3	CYN	O	575	4	1,1,1	0.52	0	-		
5	NNO	P	550	4	11,11,11	1.93	4 (36%)	11,15,15	1.69	2 (18%)
5	NNO	N	550	4	11,11,11	2.19	4 (36%)	11,15,15	1.42	2 (18%)
5	NNO	M	550	4	11,11,11	2.04	2 (18%)	11,15,15	1.32	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	NNO	O3-N1	-5.62	1.26	1.37
5	Q	550	NNO	O3-N1	-5.48	1.26	1.37
5	M	550	NNO	O3-N1	-5.17	1.27	1.37
5	O	550	NNO	O3-N1	-5.01	1.27	1.37
5	P	550	NNO	O3-N1	-4.62	1.28	1.37
5	R	550	NNO	O3-N1	-4.61	1.28	1.37
5	O	550	NNO	O2-C7	-2.99	1.21	1.30
5	N	550	NNO	O2-C7	-2.55	1.22	1.30
5	O	550	NNO	C2-C3	2.40	1.42	1.39
5	P	550	NNO	C3-C7	2.36	1.54	1.49
5	N	550	NNO	C2-C3	2.25	1.42	1.39
5	N	550	NNO	C3-C7	2.22	1.54	1.49
5	R	550	NNO	C3-C7	2.14	1.54	1.49
5	P	550	NNO	O2-C7	-2.09	1.24	1.30
5	P	550	NNO	C2-N1	-2.05	1.31	1.35
5	R	550	NNO	O2-C7	-2.04	1.24	1.30
5	Q	550	NNO	C3-C7	2.04	1.53	1.49
5	M	550	NNO	O2-C7	-2.01	1.24	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	550	NNO	O2-C7-C3	3.46	123.71	114.84
5	O	550	NNO	O2-C7-O1	-3.22	116.44	123.35
5	N	550	NNO	O2-C7-O1	-3.00	116.91	123.35
5	P	550	NNO	O2-C7-C3	2.92	122.34	114.84
5	P	550	NNO	O2-C7-O1	-2.88	117.17	123.35
5	R	550	NNO	O2-C7-O1	-2.83	117.26	123.35
5	R	550	NNO	O2-C7-C3	2.59	121.49	114.84
5	N	550	NNO	O2-C7-C3	2.47	121.18	114.84
5	M	550	NNO	O2-C7-C3	2.35	120.88	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	550	NNO	O2-C7-O1	-2.30	118.41	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	575	CYN	1	0
3	Q	575	CYN	1	0
3	M	575	CYN	1	0
3	R	575	CYN	1	0
3	O	575	CYN	1	0
5	M	550	NNO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.