



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:00 PM UTC

PDB ID : 3PCL / pdb_00003pcl
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 2-HYDROXYISONICOTINIC ACID N-OXIDE AND
CYANIDE
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-07-18
Resolution : 2.15 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

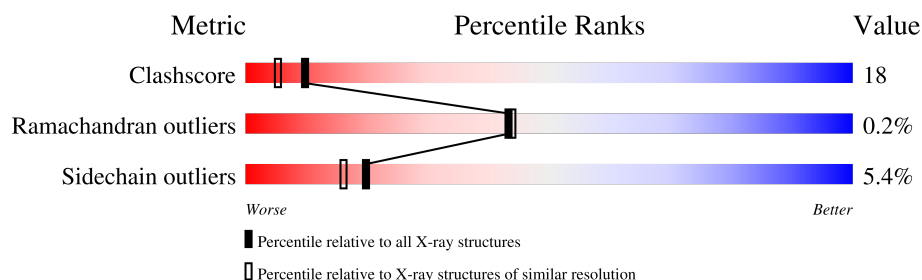
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYN	Q	575	-	-	X	-
3	CYN	R	575	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21960 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.

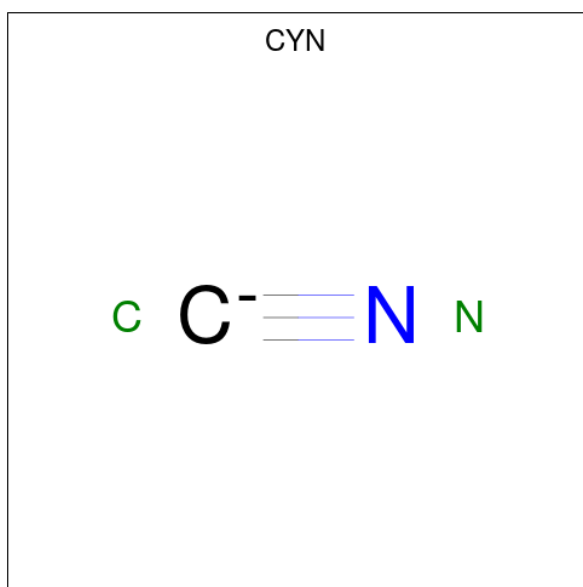
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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).

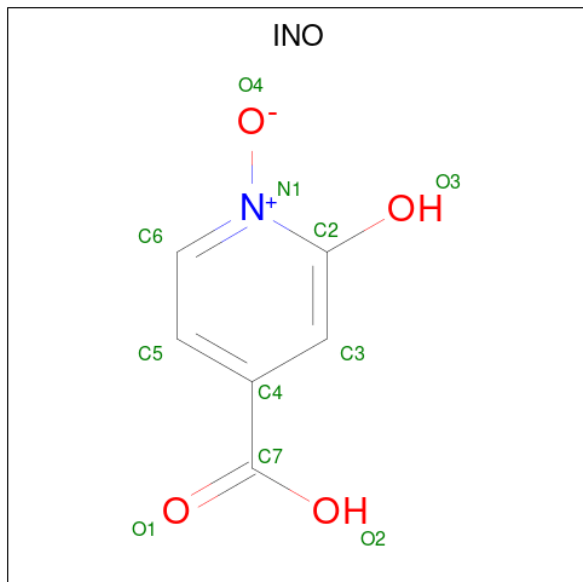


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

- 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 2-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: INO) (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	76	Total	O	0	0
			76	76		
6	M	156	Total	O	0	0
			156	156		
6	B	78	Total	O	0	0
			78	78		
6	N	159	Total	O	0	0
			159	159		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	79	Total 79	O 79	0	0
6	O	157	Total 157	O 157	0	0
6	D	78	Total 78	O 78	0	0
6	P	152	Total 152	O 152	0	0
6	E	76	Total 76	O 76	0	0
6	Q	165	Total 165	O 165	0	0
6	F	82	Total 82	O 82	0	0
6	R	152	Total 152	O 152	0	0

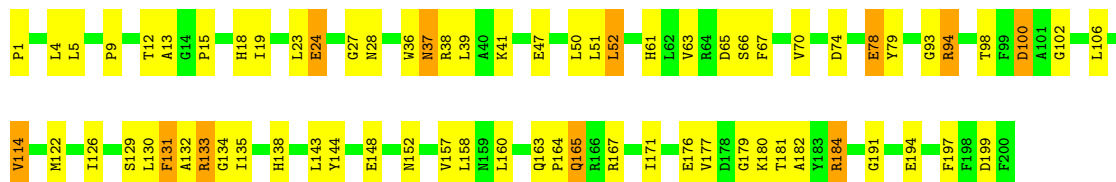
3 Residue-property plots

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.

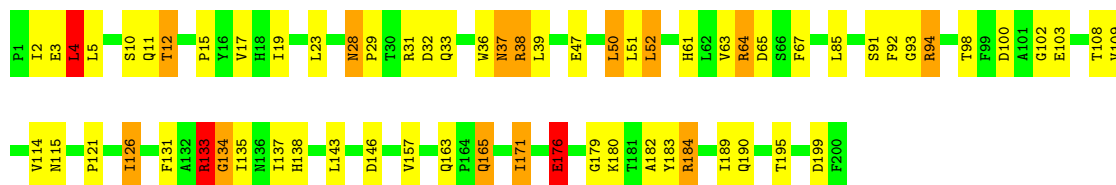
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



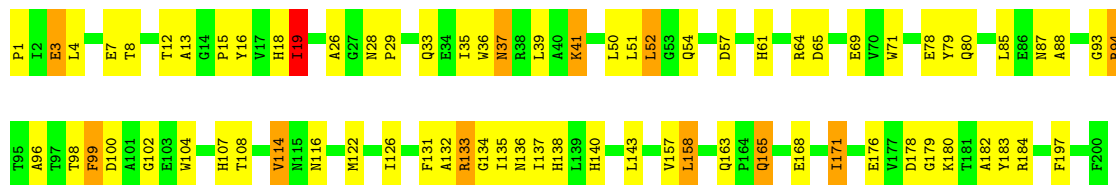
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



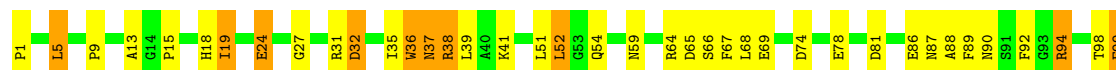
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 

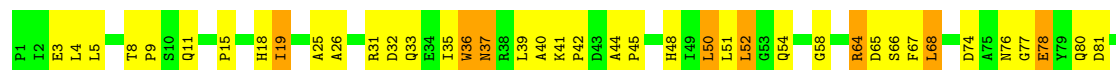




• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

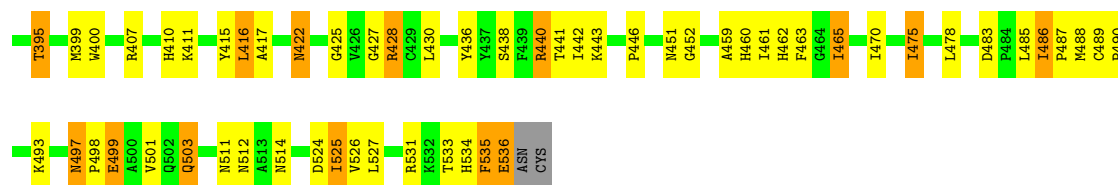


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

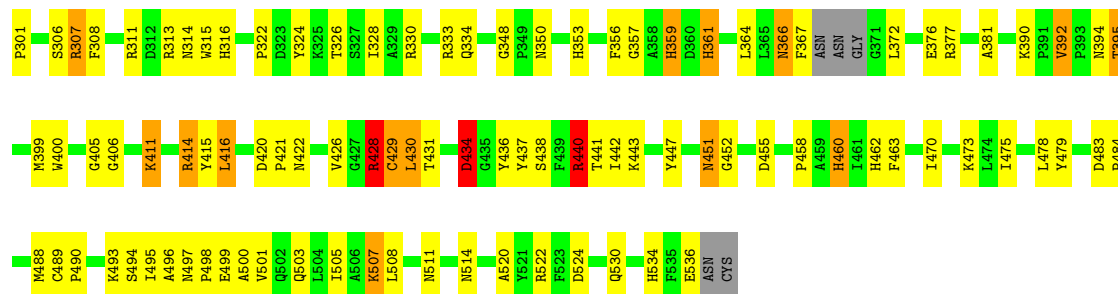


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

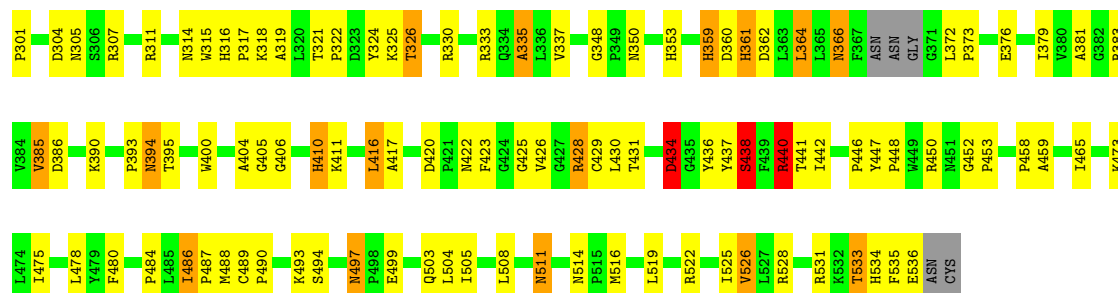




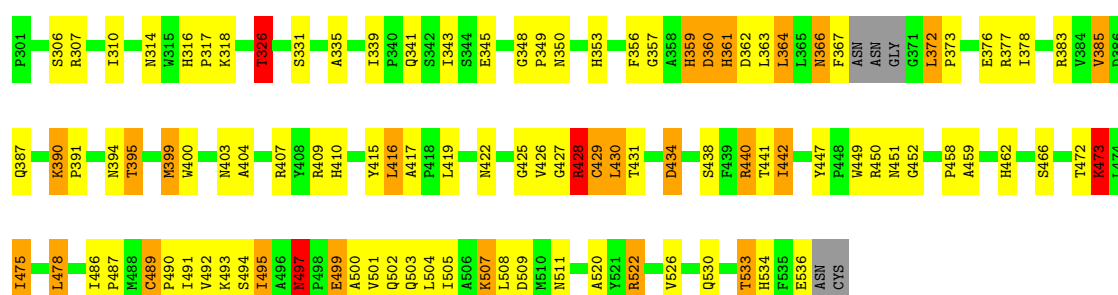
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



P301	R394	T395	M399	W400	G405	G406	R407	Y408	K411	Y415	L416	A417	F423	G424	G425	V426	G427	R428	C429	L430	T431	D434	G435	Y436	Y437	S438	F439	R440	T441	I442	K443	P444	Y447	R450	N451	G452	P453	N454	R457	P458	A459	H462	I465	S466	G467	T472	K473	L474
I475	T476	Q477	L478	D483	P484	L485	T486	P487	M488	C489	P490	S494	I495	A496	N497	P498	E499	A500	V501	Q502	Q503	K507	N514	P515	M516	R522	F523	D524	I525	V526	L527	R528	G529	Q530	R531	K532	T533	H534	F535	E536	ASN	CYS						

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	195.70 Å 128.00 Å 134.20 Å 90.00° 97.80° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.0 (6.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21960	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: FE, CYN, INO

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	1.30	2/1611 (0.1%)	1.86	30/2195 (1.4%)
1	B	1.33	7/1611 (0.4%)	1.92	33/2195 (1.5%)
1	C	1.31	2/1611 (0.1%)	1.86	30/2195 (1.4%)
1	D	1.34	6/1611 (0.4%)	1.81	22/2195 (1.0%)
1	E	1.31	2/1611 (0.1%)	1.84	34/2195 (1.5%)
1	F	1.41	5/1611 (0.3%)	1.88	32/2195 (1.5%)
2	M	1.45	6/1895 (0.3%)	1.93	43/2580 (1.7%)
2	N	1.48	8/1895 (0.4%)	1.95	52/2580 (2.0%)
2	O	1.51	7/1895 (0.4%)	2.00	50/2580 (1.9%)
2	P	1.50	14/1895 (0.7%)	1.95	50/2580 (1.9%)
2	Q	1.49	9/1895 (0.5%)	2.01	59/2580 (2.3%)
2	R	1.49	9/1895 (0.5%)	1.97	46/2580 (1.8%)
All	All	1.42	77/21036 (0.4%)	1.92	481/28650 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	313	ARG	NE-CZ	9.09	1.43	1.33
2	Q	428	ARG	CD-NE	-8.00	1.35	1.46
1	F	135	ILE	CA-CB	7.73	1.62	1.53
2	Q	441	THR	CA-CB	7.22	1.63	1.54
2	O	428	ARG	CD-NE	-7.16	1.36	1.46
2	N	486	ILE	CA-CB	7.15	1.57	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	401	GLN	N-CA	7.12	1.54	1.46
2	O	451	ASN	CA-C	7.08	1.56	1.52
1	D	135	ILE	CA-CB	6.94	1.62	1.53
2	P	440	ARG	CD-NE	-6.80	1.36	1.46
1	C	8	THR	CA-CB	6.75	1.63	1.53
2	N	441	THR	CA-CB	6.69	1.62	1.54
1	B	94	ARG	CD-NE	-6.65	1.36	1.46
2	P	428	ARG	CD-NE	-6.64	1.36	1.46
2	N	452	GLY	N-CA	6.58	1.53	1.44
2	R	467	GLY	N-CA	6.56	1.53	1.44
1	A	94	ARG	CD-NE	-6.54	1.37	1.46
1	B	195	THR	CA-CB	6.36	1.63	1.53
1	B	11	GLN	N-CA	6.21	1.53	1.45
1	D	133	ARG	N-CA	6.18	1.54	1.46
1	D	2	ILE	CA-CB	6.17	1.62	1.54
2	P	333	ARG	CD-NE	6.06	1.54	1.46
2	P	441	THR	CA-CB	6.06	1.61	1.53
1	B	11	GLN	C-O	6.05	1.31	1.23
2	P	486	ILE	CA-CB	6.03	1.57	1.54
2	R	476	THR	CA-CB	6.01	1.61	1.53
1	B	133	ARG	CD-NE	-6.00	1.37	1.46
1	A	133	ARG	CD-NE	-5.99	1.37	1.46
2	M	463	PHE	N-CA	5.92	1.53	1.45
1	F	122	MET	N-CA	5.90	1.52	1.45
2	Q	452	GLY	N-CA	5.87	1.52	1.44
2	P	525	ILE	CA-CB	5.78	1.62	1.54
2	R	533	THR	N-CA	5.77	1.53	1.45
1	B	108	THR	CA-CB	5.74	1.62	1.54
2	P	465	ILE	CA-CB	5.72	1.61	1.54
2	Q	326	THR	CA-CB	5.71	1.63	1.53
2	M	453	PRO	C-O	5.69	1.31	1.24
1	E	108	THR	CA-CB	5.69	1.62	1.54
1	D	94	ARG	CD-NE	-5.68	1.38	1.46
2	P	528	ARG	NE-CZ	5.67	1.39	1.33
2	N	478	LEU	CA-C	5.63	1.59	1.52
2	M	460	HIS	N-CA	5.60	1.52	1.46
2	Q	318	LYS	N-CA	5.60	1.52	1.45
2	R	452	GLY	N-CA	5.55	1.52	1.44
2	M	467	GLY	N-CA	5.49	1.52	1.44
2	P	379	ILE	C-O	5.43	1.30	1.24
1	F	106	LEU	N-CA	5.39	1.52	1.46
1	B	12	THR	CA-CB	5.36	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	LEU	N-CA	5.34	1.52	1.46
2	N	475	ILE	CA-C	5.33	1.59	1.52
2	P	321	THR	N-CA	5.32	1.52	1.46
2	Q	495	ILE	CA-CB	5.31	1.59	1.53
2	P	475	ILE	CA-C	5.30	1.59	1.52
2	N	336	LEU	N-CA	5.29	1.52	1.46
1	D	10	SER	CA-CB	5.25	1.61	1.53
2	O	451	ASN	CA-CB	-5.24	1.47	1.53
2	N	446	PRO	CA-C	5.24	1.58	1.52
2	R	313	ARG	CD-NE	5.24	1.53	1.46
2	Q	508	LEU	N-CA	5.23	1.52	1.46
2	R	395	THR	N-CA	5.23	1.51	1.45
2	R	533	THR	CB-OG1	5.20	1.52	1.43
2	N	307	ARG	CA-C	5.18	1.58	1.52
1	F	114	VAL	C-O	5.17	1.29	1.24
2	R	483	ASP	N-CA	5.17	1.54	1.46
2	O	460	HIS	N-CA	5.15	1.52	1.45
2	Q	472	THR	CB-OG1	5.11	1.51	1.43
2	P	337	VAL	N-CA	5.10	1.52	1.46
1	E	196	VAL	CA-C	5.09	1.58	1.52
2	M	375	GLY	N-CA	5.07	1.50	1.45
2	Q	310	ILE	CA-CB	5.07	1.60	1.54
1	F	36	TRP	CA-C	-5.06	1.48	1.53
2	P	324	TYR	CA-C	5.05	1.59	1.53
2	P	326	THR	CA-CB	5.03	1.61	1.53
2	O	429	CYS	N-CA	5.02	1.52	1.46
2	R	529	GLY	N-CA	5.02	1.52	1.45
1	C	108	THR	CA-CB	5.01	1.61	1.54
2	O	441	THR	CA-CB	5.01	1.60	1.54

All (481) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	428	ARG	CD-NE-CZ	18.09	149.72	124.40
1	A	94	ARG	CD-NE-CZ	16.75	147.86	124.40
1	B	133	ARG	CD-NE-CZ	15.78	146.49	124.40
2	O	428	ARG	CD-NE-CZ	14.94	145.31	124.40
1	B	94	ARG	CD-NE-CZ	14.76	145.06	124.40
1	A	133	ARG	CD-NE-CZ	12.48	141.87	124.40
2	Q	434	ASP	CA-CB-CG	-12.32	100.28	112.60
2	O	353	HIS	CA-CB-CG	-11.13	102.67	113.80
2	N	428	ARG	CD-NE-CZ	11.09	139.92	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	NE-CZ-NH2	-10.81	109.47	119.20
2	N	452	GLY	N-CA-C	-10.73	99.24	112.23
2	O	434	ASP	CA-CB-CG	-10.68	101.92	112.60
1	B	176	GLU	CB-CG-CD	10.47	130.40	112.60
2	M	452	GLY	N-CA-C	-10.30	99.77	112.23
2	Q	452	GLY	N-CA-C	-10.15	99.95	112.23
2	O	452	GLY	N-CA-C	-9.75	100.43	112.23
2	N	361	HIS	CA-CB-CG	-9.73	104.07	113.80
1	A	184	ARG	CD-NE-CZ	9.69	137.96	124.40
2	N	440	ARG	NE-CZ-NH2	-9.66	110.50	119.20
2	O	463	PHE	CA-CB-CG	9.64	123.44	113.80
2	P	372	LEU	CB-CA-C	9.59	122.01	108.68
1	B	133	ARG	NE-CZ-NH1	9.43	130.93	121.50
2	O	451	ASN	O-C-N	9.43	129.19	120.71
1	A	94	ARG	CG-CD-NE	9.19	132.21	112.00
2	R	361	HIS	CA-CB-CG	-9.10	104.70	113.80
1	D	94	ARG	NE-CZ-NH2	-9.02	111.08	119.20
1	E	90	ASN	CA-CB-CG	8.97	121.57	112.60
1	F	94	ARG	CD-NE-CZ	8.95	136.93	124.40
2	M	353	HIS	CA-CB-CG	-8.88	104.92	113.80
2	R	454	ASN	CA-CB-CG	8.87	121.47	112.60
1	F	133	ARG	CD-NE-CZ	-8.73	112.18	124.40
1	F	127	ASN	CA-CB-CG	-8.54	104.06	112.60
1	D	94	ARG	CD-NE-CZ	8.51	136.32	124.40
1	A	94	ARG	CB-CG-CD	8.50	130.84	111.30
2	M	361	HIS	CA-CB-CG	-8.42	105.38	113.80
2	P	428	ARG	CG-CD-NE	8.42	130.52	112.00
1	B	133	ARG	NE-CZ-NH2	-8.24	111.79	119.20
1	C	87	ASN	CA-CB-CG	8.22	120.82	112.60
1	B	94	ARG	CG-CD-NE	8.22	130.08	112.00
1	A	94	ARG	NE-CZ-NH1	8.20	129.70	121.50
2	Q	440	ARG	NE-CZ-NH2	-8.20	111.82	119.20
1	C	37	ASN	N-CA-C	8.05	122.47	113.21
1	A	133	ARG	N-CA-CB	-7.97	97.79	109.83
2	Q	361	HIS	CA-CB-CG	-7.96	105.84	113.80
2	N	514	ASN	O-C-N	7.93	129.24	120.83
2	O	316	HIS	CA-CB-CG	-7.92	105.88	113.80
1	F	64	ARG	NE-CZ-NH1	-7.90	113.60	121.50
1	F	66	SER	N-CA-CB	7.87	121.50	110.17
1	F	64	ARG	CD-NE-CZ	-7.84	113.42	124.40
1	F	94	ARG	NE-CZ-NH1	7.84	129.34	121.50
1	D	37	ASN	N-CA-C	7.80	121.66	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	428	ARG	CD-NE-CZ	7.66	135.13	124.40
2	M	440	ARG	NE-CZ-NH2	-7.59	112.37	119.20
2	R	457	ARG	CD-NE-CZ	7.58	135.02	124.40
2	N	333	ARG	N-CA-C	-7.58	104.27	113.97
2	P	333	ARG	CD-NE-CZ	-7.58	113.79	124.40
2	M	372	LEU	CB-CA-C	7.57	119.13	108.76
1	E	37	ASN	N-CA-C	7.52	121.86	113.21
2	P	494	SER	N-CA-C	-7.50	103.39	112.54
1	F	90	ASN	CA-CB-CG	7.46	120.06	112.60
1	B	37	ASN	N-CA-C	7.44	121.94	113.02
2	Q	348	GLY	O-C-N	7.43	129.21	121.77
2	R	434	ASP	CA-CB-CG	-7.41	105.19	112.60
2	P	428	ARG	CB-CG-CD	7.40	128.33	111.30
1	A	37	ASN	N-CA-C	7.40	121.21	112.93
2	Q	353	HIS	CA-CB-CG	-7.39	106.41	113.80
2	R	450	ARG	CD-NE-CZ	-7.36	114.09	124.40
1	E	136	ASN	O-C-N	7.32	129.61	122.07
2	M	486	ILE	O-C-N	7.32	125.10	120.42
2	M	422	ASN	OD1-CG-ND2	7.26	129.86	122.60
2	O	428	ARG	CG-CD-NE	7.21	127.86	112.00
1	C	140	HIS	CA-CB-CG	7.19	120.99	113.80
1	D	171	ILE	N-CA-C	7.13	118.40	107.99
2	O	314	ASN	CA-CB-CG	-7.11	105.49	112.60
2	R	522	ARG	CD-NE-CZ	-7.11	114.45	124.40
2	O	366	ASN	N-CA-C	7.10	121.53	113.01
1	B	94	ARG	CB-CG-CD	7.09	127.62	111.30
2	P	440	ARG	CD-NE-CZ	7.06	134.28	124.40
2	Q	339	ILE	O-C-N	7.04	126.12	121.69
2	O	475	ILE	N-CA-CB	7.02	121.10	111.41
1	D	94	ARG	NE-CZ-NH1	7.01	128.51	121.50
2	N	350	ASN	CA-CB-CG	-7.01	105.59	112.60
1	E	158	LEU	CB-CA-C	7.01	122.42	110.79
2	Q	417	ALA	CB-CA-C	7.01	119.56	109.26
2	N	407	ARG	CD-NE-CZ	-6.97	114.65	124.40
1	F	5	LEU	O-C-N	6.96	129.22	121.43
2	R	522	ARG	NE-CZ-NH1	-6.95	114.55	121.50
2	N	486	ILE	O-C-N	6.93	124.85	120.42
2	P	353	HIS	CA-CB-CG	-6.92	106.88	113.80
2	O	514	ASN	CA-CB-CG	6.92	119.52	112.60
1	C	107	HIS	CA-CB-CG	-6.91	106.89	113.80
2	P	504	LEU	CA-C-N	-6.89	113.75	122.37
2	P	504	LEU	C-N-CA	-6.89	113.75	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	451	ASN	CA-C-O	-6.88	115.35	119.55
1	D	5	LEU	N-CA-C	-6.87	101.10	109.83
1	E	99	PHE	CA-CB-CG	6.85	120.65	113.80
2	P	326	THR	CA-CB-OG1	-6.81	99.38	109.60
1	F	11	GLN	O-C-N	6.81	131.02	123.25
2	M	494	SER	N-CA-C	-6.81	104.24	112.54
2	P	361	HIS	CA-CB-CG	-6.76	107.04	113.80
2	M	431	THR	N-CA-C	-6.75	101.62	110.53
2	Q	341	GLN	OE1-CD-NE2	6.74	129.34	122.60
2	R	440	ARG	NE-CZ-NH2	-6.74	113.13	119.20
2	O	316	HIS	O-C-N	6.73	128.74	121.60
1	F	165	GLN	CB-CG-CD	6.69	123.98	112.60
2	M	459	ALA	N-CA-C	-6.69	100.53	110.23
1	A	5	LEU	N-CA-C	-6.68	101.34	109.83
2	P	420	ASP	CB-CA-C	6.67	117.82	110.15
1	E	133	ARG	CA-CB-CG	6.64	127.39	114.10
2	N	503	GLN	CA-CB-CG	6.63	127.36	114.10
2	N	499	GLU	CB-CG-CD	6.63	123.87	112.60
1	B	94	ARG	NE-CZ-NH1	6.62	128.12	121.50
1	E	133	ARG	N-CA-C	-6.61	100.64	110.23
2	R	367	PHE	CA-C-O	-6.61	109.56	120.80
2	R	314	ASN	N-CA-C	-6.60	105.14	113.72
2	P	359	HIS	CA-CB-CG	-6.58	107.22	113.80
2	P	531	ARG	CA-CB-CG	6.58	127.26	114.10
2	P	348	GLY	O-C-N	6.58	128.35	121.77
2	N	465	ILE	O-C-N	6.57	129.80	123.03
2	Q	387	GLN	O-C-N	6.57	130.93	122.39
2	M	514	ASN	CB-CA-C	6.55	116.66	110.17
2	P	434	ASP	CA-CB-CG	-6.55	106.05	112.60
2	R	443	LYS	O-C-N	6.54	127.12	121.30
1	B	38	ARG	CD-NE-CZ	-6.54	115.25	124.40
2	P	383	ARG	CD-NE-CZ	-6.52	115.27	124.40
2	Q	385	VAL	O-C-N	6.52	130.17	123.00
2	P	511	ASN	CA-CB-CG	6.51	119.11	112.60
1	B	47	GLU	CB-CG-CD	6.50	123.65	112.60
2	P	452	GLY	N-CA-C	-6.50	99.08	112.34
2	Q	466	SER	N-CA-C	6.49	118.23	111.03
2	M	348	GLY	O-C-N	6.44	128.21	121.77
2	P	366	ASN	N-CA-C	6.44	120.73	113.01
1	E	5	LEU	N-CA-C	-6.42	101.22	110.08
1	C	183	TYR	N-CA-CB	6.42	120.85	110.77
1	B	10	SER	CA-C-O	-6.42	114.24	121.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	ASP	CA-CB-CG	-6.41	106.19	112.60
1	A	94	ARG	NE-CZ-NH2	-6.41	113.44	119.20
2	M	333	ARG	CD-NE-CZ	-6.38	115.47	124.40
2	N	314	ASN	CB-CA-C	6.38	120.90	109.29
1	B	134	GLY	N-CA-C	-6.37	106.93	115.21
2	O	440	ARG	CA-C-O	-6.36	113.26	120.32
1	E	36	TRP	N-CA-C	6.33	116.80	108.07
2	N	353	HIS	CA-CB-CG	-6.32	107.48	113.80
1	E	127	ASN	OD1-CG-ND2	6.32	128.92	122.60
1	A	131	PHE	CA-CB-CG	6.30	120.10	113.80
1	E	38	ARG	CD-NE-CZ	-6.30	115.58	124.40
2	O	414	ARG	CD-NE-CZ	-6.30	115.58	124.40
1	E	59	ASN	CA-CB-CG	-6.28	106.32	112.60
2	O	520	ALA	O-C-N	6.28	130.42	123.33
2	R	314	ASN	N-CA-CB	6.28	119.88	110.65
2	M	422	ASN	CA-CB-CG	-6.27	106.33	112.60
1	E	189	ILE	O-C-N	6.26	127.95	121.87
2	P	459	ALA	N-CA-C	-6.26	100.77	110.10
2	O	430	LEU	N-CA-CB	-6.26	99.94	110.83
2	M	339	ILE	O-C-N	6.23	128.20	121.10
1	D	76	ASN	CA-CB-CG	-6.22	106.38	112.60
2	Q	367	PHE	CA-C-O	-6.22	110.22	120.80
2	Q	366	ASN	N-CA-C	6.22	120.59	113.19
1	B	133	ARG	CA-CB-CG	6.21	126.53	114.10
2	M	417	ALA	N-CA-C	-6.21	102.23	109.93
1	B	94	ARG	NE-CZ-NH2	-6.21	113.61	119.20
2	O	494	SER	N-CA-C	-6.19	104.99	112.54
2	O	440	ARG	O-C-N	6.19	130.55	123.31
1	F	188	ARG	CB-CA-C	6.19	120.33	110.19
1	A	23	LEU	CB-CA-C	6.18	121.09	110.84
2	M	411	LYS	CB-CA-C	-6.18	100.49	110.74
2	O	443	LYS	O-C-N	6.17	126.92	121.18
2	P	393	PRO	CA-C-N	6.17	131.15	122.46
2	P	393	PRO	C-N-CA	6.17	131.15	122.46
2	R	514	ASN	O-C-N	6.16	126.98	121.19
2	O	440	ARG	NE-CZ-NH2	-6.15	113.67	119.20
2	O	359	HIS	CA-CB-CG	-6.15	107.65	113.80
2	N	443	LYS	O-C-N	6.14	126.89	121.18
2	N	475	ILE	N-CA-CB	6.13	120.47	111.52
2	M	428	ARG	CD-NE-CZ	6.13	132.98	124.40
1	D	133	ARG	CD-NE-CZ	6.12	132.97	124.40
2	P	526	VAL	O-C-N	6.09	130.23	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	430	LEU	N-CA-CB	-6.09	101.01	110.57
1	C	96	ALA	N-CA-CB	-6.05	101.62	111.24
2	O	361	HIS	CA-CB-CG	-6.04	107.76	113.80
1	F	11	GLN	CA-C-O	-6.04	114.81	121.33
2	O	367	PHE	CA-C-O	-6.03	110.55	120.80
1	F	5	LEU	CA-C-O	-6.03	113.74	120.25
2	R	366	ASN	CA-C-O	-6.02	111.90	120.51
2	R	507	LYS	CG-CD-CE	6.00	125.11	111.30
2	P	385	VAL	O-C-N	6.00	129.60	123.00
1	C	69	GLU	CB-CG-CD	6.00	122.80	112.60
1	C	99	PHE	CA-CB-CG	6.00	119.80	113.80
1	F	171	ILE	N-CA-C	6.00	116.44	107.51
1	F	37	ASN	N-CA-C	6.00	120.21	113.02
1	E	88	ALA	N-CA-C	-5.99	104.68	112.23
1	A	47	GLU	CB-CG-CD	5.99	122.79	112.60
2	P	324	TYR	O-C-N	5.99	129.94	122.63
2	N	384	VAL	O-C-N	5.99	130.11	123.10
1	F	68	LEU	N-CA-CB	-5.99	100.48	111.37
1	D	24	GLU	CB-CG-CD	5.98	122.76	112.60
1	B	5	LEU	N-CA-C	-5.97	101.84	110.08
1	F	106	LEU	N-CA-CB	-5.95	100.35	111.13
1	E	94	ARG	NE-CZ-NH1	5.95	127.45	121.50
2	Q	533	THR	N-CA-C	-5.93	101.70	110.48
1	B	64	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	C	178	ASP	CA-CB-CG	-5.92	106.68	112.60
1	F	158	LEU	CB-CA-C	5.92	120.62	110.79
2	Q	492	VAL	O-C-N	5.91	127.70	121.91
2	R	494	SER	N-CA-C	-5.91	105.33	112.54
1	A	167	ARG	CD-NE-CZ	-5.91	116.13	124.40
2	O	348	GLY	O-C-N	5.91	127.68	121.77
1	E	183	TYR	O-C-N	5.91	130.22	123.31
2	R	311	ARG	CA-C-O	-5.91	115.12	121.56
2	N	422	ASN	CA-CB-CG	-5.91	106.69	112.60
1	C	171	ILE	N-CA-C	5.91	116.61	107.99
2	P	534	HIS	CA-CB-CG	5.89	119.69	113.80
2	Q	359	HIS	CA-CB-CG	-5.89	107.91	113.80
2	Q	499	GLU	CB-CG-CD	5.89	122.61	112.60
2	N	357	GLY	N-CA-C	-5.87	105.03	112.54
2	P	422	ASN	CA-CB-CG	-5.87	106.73	112.60
2	M	320	LEU	O-C-N	5.87	130.03	123.05
2	P	322	PRO	N-CA-C	5.86	122.31	113.81
2	M	450	ARG	CD-NE-CZ	5.84	132.58	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	N-CA-CB	-5.84	101.00	109.83
2	Q	339	ILE	N-CA-C	-5.84	104.40	109.19
2	M	480	PHE	CA-CB-CG	-5.84	107.96	113.80
1	E	64	ARG	CD-NE-CZ	-5.83	116.23	124.40
1	F	133	ARG	N-CA-C	-5.83	102.03	110.24
1	F	190	GLN	N-CA-CB	-5.83	102.53	111.56
2	O	322	PRO	CB-CA-C	5.82	121.17	111.56
2	Q	475	ILE	N-CA-CB	5.81	119.43	111.41
2	O	524	ASP	CA-CB-CG	-5.81	106.79	112.60
2	O	496	ALA	N-CA-C	5.80	118.38	111.71
1	C	137	ILE	CB-CA-C	5.80	118.79	110.33
2	Q	372	LEU	CB-CA-C	5.79	117.55	108.63
2	Q	385	VAL	CA-C-O	-5.79	115.76	121.67
2	N	459	ALA	N-CA-C	-5.78	101.49	110.10
2	R	357	GLY	N-CA-C	-5.78	105.98	112.33
1	F	133	ARG	CA-CB-CG	5.77	125.64	114.10
2	Q	428	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	A	197	PHE	N-CA-C	-5.76	100.40	109.50
1	A	177	VAL	O-C-N	5.76	128.61	123.03
2	N	307	ARG	O-C-N	5.75	130.29	123.27
2	O	394	ASN	CA-C-O	-5.74	115.18	121.84
1	A	38	ARG	CD-NE-CZ	-5.73	116.37	124.40
1	B	137	ILE	CB-CA-C	5.72	118.68	110.33
1	C	41	LYS	N-CA-C	-5.71	102.85	109.93
1	E	123	ALA	N-CA-C	-5.71	101.90	109.84
2	N	470	ILE	N-CA-C	-5.71	104.05	112.04
1	A	18	HIS	CA-CB-CG	-5.70	108.11	113.80
1	C	19	ILE	N-CA-CB	5.70	117.59	110.47
1	F	78	GLU	N-CA-CB	5.69	119.86	110.69
2	O	377	ARG	CA-C-N	-5.69	114.61	122.69
2	O	377	ARG	C-N-CA	-5.69	114.61	122.69
2	M	315	TRP	N-CA-C	-5.67	104.48	111.40
1	D	68	LEU	O-C-N	5.67	130.19	123.27
1	A	184	ARG	NE-CZ-NH2	-5.66	114.11	119.20
2	N	497	ASN	CB-CA-C	5.65	116.58	110.08
2	Q	422	ASN	CA-CB-CG	-5.65	106.95	112.60
2	P	333	ARG	CB-CA-C	5.65	119.57	109.29
2	O	330	ARG	NE-CZ-NH2	-5.64	114.12	119.20
2	M	451	ASN	OD1-CG-ND2	5.64	128.24	122.60
1	B	157	VAL	CB-CA-C	5.64	119.42	112.04
1	B	184	ARG	NE-CZ-NH2	-5.64	114.13	119.20
2	N	306	SER	CA-C-N	5.63	131.84	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	306	SER	C-N-CA	5.63	131.84	122.73
2	O	422	ASN	CA-CB-CG	-5.62	106.97	112.60
2	R	407	ARG	NE-CZ-NH1	5.62	127.12	121.50
2	M	440	ARG	NH1-CZ-NH2	5.61	126.59	119.30
2	N	535	PHE	CA-CB-CG	5.61	119.41	113.80
2	O	311	ARG	N-CA-CB	5.61	118.25	110.17
2	Q	438	SER	N-CA-CB	5.61	120.15	111.24
1	D	94	ARG	CG-CD-NE	5.60	124.33	112.00
2	R	304	ASP	CA-CB-CG	-5.60	107.00	112.60
1	E	181	THR	N-CA-CB	5.59	118.35	109.51
1	E	112	GLY	N-CA-C	-5.59	103.85	112.85
1	D	133	ARG	N-CA-CB	-5.59	100.82	109.48
2	N	430	LEU	N-CA-CB	-5.57	101.72	110.69
1	A	74	ASP	N-CA-C	-5.56	102.67	110.35
2	R	459	ALA	N-CA-C	-5.56	102.16	110.23
2	M	491	ILE	N-CA-CB	5.55	118.91	110.58
2	R	346	THR	CA-CB-OG1	-5.55	101.27	109.60
2	R	350	ASN	N-CA-CB	5.55	119.26	110.55
2	N	307	ARG	CA-C-O	-5.54	114.28	120.66
2	M	526	VAL	O-C-N	5.54	129.58	123.10
2	N	497	ASN	CA-C-O	5.54	122.89	119.29
2	M	420	ASP	O-C-N	5.54	127.43	121.12
2	P	475	ILE	O-C-N	5.53	129.23	123.26
1	E	81	ASP	N-CA-C	5.52	119.18	112.23
2	M	402	ALA	O-C-N	5.52	129.04	122.20
2	O	501	VAL	O-C-N	5.50	127.44	121.94
2	Q	522	ARG	CD-NE-CZ	-5.50	116.71	124.40
2	O	430	LEU	CB-CA-C	5.49	119.86	109.37
2	Q	458	PRO	N-CA-C	-5.49	103.48	111.33
2	Q	383	ARG	CD-NE-CZ	-5.49	116.72	124.40
2	P	533	THR	CA-C-O	-5.49	115.58	121.56
1	F	181	THR	N-CA-CB	5.48	118.02	109.85
1	C	57	ASP	CA-CB-CG	5.48	118.08	112.60
2	Q	497	ASN	CB-CA-C	5.48	117.27	109.38
1	F	162	GLU	N-CA-C	5.47	117.24	111.28
2	Q	473	LYS	CB-CA-C	5.45	118.47	109.70
1	D	92	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	133	ARG	NE-CZ-NH2	-5.44	114.30	119.20
1	F	5	LEU	N-CA-C	-5.44	102.92	109.83
1	A	184	ARG	O-C-N	5.44	129.42	123.27
2	R	533	THR	CA-CB-OG1	-5.44	101.44	109.60
2	M	434	ASP	CA-CB-CG	-5.44	107.16	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	423	PHE	CA-CB-CG	-5.44	108.36	113.80
2	O	458	PRO	N-CA-C	-5.44	102.91	111.34
2	Q	501	VAL	N-CA-CB	5.44	116.91	110.55
2	N	536	GLU	CA-C-O	5.43	130.04	120.80
2	Q	511	ASN	OD1-CG-ND2	5.43	128.03	122.60
2	R	417	ALA	N-CA-C	-5.43	102.59	110.08
2	Q	459	ALA	N-CA-C	-5.43	102.01	110.10
2	M	489	CYS	O-C-N	5.42	126.22	121.18
2	M	440	ARG	CD-NE-CZ	-5.42	116.82	124.40
2	R	353	HIS	CA-CB-CG	-5.42	108.38	113.80
2	Q	428	ARG	CG-CD-NE	5.41	123.91	112.00
1	E	94	ARG	CG-CD-NE	5.41	123.90	112.00
2	M	366	ASN	N-CA-C	5.41	120.83	113.37
1	E	127	ASN	CA-CB-CG	-5.41	107.19	112.60
1	C	69	GLU	N-CA-CB	5.41	120.79	111.00
2	N	308	PHE	CB-CA-C	5.40	119.68	109.37
1	C	3	GLU	CA-C-O	-5.40	114.87	120.70
2	M	455	ASP	O-C-N	5.40	129.50	123.19
2	O	508	LEU	CA-C-O	-5.40	114.77	120.92
1	D	150	GLN	O-C-N	5.39	127.91	122.09
1	B	17	VAL	CA-C-N	5.39	127.77	120.38
1	B	17	VAL	C-N-CA	5.39	127.77	120.38
2	Q	360	ASP	CB-CA-C	5.39	119.74	110.79
1	E	132	ALA	O-C-N	5.39	128.32	123.26
1	B	64	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	B	176	GLU	CG-CD-OE1	5.38	130.77	118.40
1	A	13	ALA	O-C-N	5.38	128.88	122.27
2	P	475	ILE	N-CA-CB	5.36	118.81	111.41
2	N	460	HIS	O-C-N	5.36	129.36	123.25
1	F	64	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	A	41	LYS	N-CA-C	-5.36	102.90	110.29
2	N	531	ARG	CD-NE-CZ	5.36	131.90	124.40
2	O	392	VAL	O-C-N	5.35	127.20	121.10
2	N	501	VAL	N-CA-CB	5.35	116.81	110.55
2	P	335	ALA	O-C-N	5.35	129.17	122.86
1	B	171	ILE	N-CA-C	5.34	115.47	107.51
2	M	357	GLY	N-CA-C	-5.34	105.45	112.82
2	P	410	HIS	CA-C-N	5.34	127.75	120.54
2	P	410	HIS	C-N-CA	5.34	127.75	120.54
1	E	196	VAL	O-C-N	5.33	128.48	122.67
2	N	451	ASN	N-CA-C	-5.32	99.46	110.80
2	N	499	GLU	CG-CD-OE1	5.32	130.64	118.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	THR	CA-C-N	5.31	130.39	123.06
1	C	108	THR	C-N-CA	5.31	130.39	123.06
2	Q	394	ASN	CA-C-O	-5.31	115.68	121.84
1	A	152	ASN	CA-CB-CG	5.31	117.91	112.60
2	M	420	ASP	CB-CA-C	5.31	116.06	110.17
2	Q	450	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	F	94	ARG	NE-CZ-NH2	-5.30	114.43	119.20
2	Q	377	ARG	NE-CZ-NH1	-5.30	116.20	121.50
2	O	350	ASN	CA-CB-CG	-5.30	107.30	112.60
2	P	514	ASN	O-C-N	5.29	126.44	120.83
2	Q	428	ARG	NE-CZ-NH1	5.29	126.79	121.50
2	N	411	LYS	CB-CA-C	-5.29	102.06	110.84
1	E	190	GLN	N-CA-C	5.29	117.29	108.99
2	Q	390	LYS	CA-C-O	5.29	124.46	119.76
2	Q	314	ASN	N-CA-C	-5.28	106.85	113.72
2	N	483	ASP	CA-C-O	5.28	124.69	119.51
2	N	512	ASN	O-C-N	5.28	128.94	122.34
2	P	394	ASN	CA-C-O	-5.27	115.86	122.03
2	N	461	ILE	O-C-N	5.27	128.95	123.26
1	D	19	ILE	CB-CA-C	5.26	119.24	112.14
2	N	485	LEU	CA-C-N	5.25	125.47	120.43
2	N	485	LEU	C-N-CA	5.25	125.47	120.43
2	P	458	PRO	CB-CA-C	-5.25	103.28	111.22
2	M	475	ILE	N-CA-CB	5.25	119.19	111.52
2	N	463	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	38	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	B	4	LEU	N-CA-CB	-5.25	100.58	110.07
1	E	94	ARG	CD-NE-CZ	5.24	131.74	124.40
2	R	380	VAL	N-CA-CB	5.24	118.06	111.46
2	M	446	PRO	N-CA-C	-5.24	103.22	111.34
2	N	524	ASP	O-C-N	5.24	129.12	123.10
2	O	313	ARG	CD-NE-CZ	-5.24	117.06	124.40
2	O	307	ARG	N-CA-C	-5.24	101.34	109.72
1	B	189	ILE	O-C-N	5.23	126.95	121.87
1	D	133	ARG	NE-CZ-NH2	-5.23	114.49	119.20
2	O	496	ALA	CA-C-O	-5.23	114.19	120.10
1	D	5	LEU	O-C-N	5.23	127.29	121.43
1	D	32	ASP	O-C-N	5.23	127.53	122.09
1	E	127	ASN	CA-C-O	-5.23	115.09	121.05
2	R	475	ILE	N-CA-CB	5.23	119.15	111.52
1	C	7	GLU	CB-CG-CD	5.23	121.48	112.60
2	P	428	ARG	NE-CZ-NH1	5.23	126.73	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	473	LYS	CA-CB-CG	5.23	124.55	114.10
1	B	189	ILE	N-CA-CB	5.22	117.64	110.54
2	P	314	ASN	N-CA-CB	5.22	118.16	110.33
1	E	159	ASN	CA-CB-CG	-5.22	107.38	112.60
1	B	126	ILE	CA-C-O	-5.22	114.91	120.39
1	B	183	TYR	N-CA-CB	5.22	119.82	110.80
1	C	94	ARG	NE-CZ-NH2	5.21	123.89	119.20
2	P	505	ILE	CB-CA-C	5.21	117.27	110.96
2	P	372	LEU	N-CA-CB	-5.21	101.51	110.11
1	B	28	ASN	O-C-N	5.21	125.89	121.20
2	P	350	ASN	CA-CB-CG	-5.21	107.39	112.60
1	B	184	ARG	CG-CD-NE	-5.21	100.55	112.00
2	Q	378	ILE	O-C-N	5.20	128.72	123.00
2	O	357	GLY	N-CA-C	-5.20	104.55	112.51
1	D	28	ASN	O-C-N	5.20	125.88	121.20
2	R	311	ARG	O-C-N	5.19	128.98	122.86
2	Q	372	LEU	N-CA-C	-5.19	102.98	110.40
2	R	394	ASN	O-C-N	5.18	129.05	122.57
2	R	489	CYS	CA-C-O	5.18	124.37	119.76
2	Q	502	GLN	OE1-CD-NE2	5.18	127.78	122.60
2	N	383	ARG	N-CA-CB	-5.17	101.96	111.37
2	N	311	ARG	N-CA-CB	5.17	117.62	110.17
2	R	314	ASN	CA-CB-CG	5.17	117.77	112.60
1	F	88	ALA	N-CA-C	-5.17	105.72	112.23
1	C	133	ARG	N-CA-C	-5.17	102.74	110.23
2	Q	451	ASN	N-CA-C	-5.17	99.80	110.80
2	O	508	LEU	O-C-N	5.16	129.35	122.95
1	E	64	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	F	112	GLY	N-CA-C	-5.15	104.55	112.85
2	M	458	PRO	CB-CA-C	-5.15	104.47	111.12
1	E	133	ARG	N-CA-CB	-5.15	102.05	109.83
2	Q	394	ASN	O-C-N	5.15	128.94	122.55
2	R	452	GLY	N-CA-C	-5.15	101.83	112.34
2	R	516	MET	CA-C-O	-5.15	114.24	120.32
1	A	148	GLU	CA-C-O	5.15	126.61	120.53
2	R	438	SER	N-CA-CB	5.15	119.43	111.24
2	N	326	THR	CA-C-O	-5.15	114.44	120.20
1	C	13	ALA	N-CA-C	-5.15	105.85	111.82
2	Q	357	GLY	CA-C-N	5.14	127.43	120.38
2	Q	357	GLY	C-N-CA	5.14	127.43	120.38
2	P	438	SER	CB-CA-C	5.14	119.57	110.16
2	O	333	ARG	CB-CA-C	5.13	118.23	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	GLU	CA-CB-CG	5.13	124.36	114.10
1	C	157	VAL	CB-CA-C	5.13	118.74	112.02
2	R	305	ASN	CB-CA-C	5.13	117.69	109.07
2	Q	494	SER	N-CA-C	-5.12	106.29	112.54
1	B	10	SER	O-C-N	5.12	128.69	122.85
1	C	114	VAL	CB-CA-C	5.12	118.71	110.82
1	E	177	VAL	CB-CA-C	5.12	117.33	110.42
2	R	314	ASN	O-C-N	5.12	128.65	122.35
2	N	451	ASN	CB-CA-C	5.12	120.60	110.42
2	N	525	ILE	O-C-N	5.11	128.57	123.10
2	P	386	ASP	CB-CA-C	5.11	119.29	110.45
2	Q	331	SER	O-C-N	5.10	126.28	121.38
2	N	534	HIS	N-CA-CB	5.10	121.01	111.52
2	Q	345	GLU	N-CA-C	5.10	119.58	112.90
2	Q	489	CYS	N-CA-C	5.10	116.96	109.42
2	Q	326	THR	CA-CB-OG1	-5.09	101.97	109.60
2	R	431	THR	N-CA-C	-5.09	103.32	110.50
2	R	502	GLN	OE1-CD-NE2	5.09	127.69	122.60
2	M	410	HIS	CA-C-N	5.07	128.43	120.82
2	M	410	HIS	C-N-CA	5.07	128.43	120.82
2	O	324	TYR	N-CA-C	-5.07	98.45	107.98
2	R	495	ILE	CB-CG1-CD1	5.07	124.44	113.80
2	N	378	ILE	O-C-N	5.06	128.74	123.02
1	E	198	PHE	O-C-N	5.06	128.75	123.03
1	E	32	ASP	O-C-N	5.06	127.49	122.08
2	O	483	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	2	ILE	CB-CA-C	-5.05	104.66	111.63
2	P	480	PHE	CA-CB-CG	-5.05	108.75	113.80
2	M	443	LYS	O-C-N	5.05	125.88	121.18
1	A	171	ILE	N-CA-C	5.04	115.35	107.99
2	Q	407	ARG	NE-CZ-NH1	5.04	126.54	121.50
2	Q	497	ASN	CA-CB-CG	5.04	117.64	112.60
1	F	124	PRO	N-CA-C	-5.04	103.18	111.15
1	A	129	SER	CA-CB-OG	5.04	121.18	111.10
1	A	133	ARG	CB-CG-CD	-5.04	99.71	111.30
2	R	452	GLY	CA-C-N	5.04	124.70	119.56
2	R	452	GLY	C-N-CA	5.04	124.70	119.56
1	F	114	VAL	CA-C-O	-5.03	115.44	121.28
2	N	385	VAL	CA-C-O	-5.03	116.39	121.67
1	A	143	LEU	O-C-N	5.03	129.20	123.27
1	C	197	PHE	N-CA-C	-5.03	101.68	109.72
2	M	415	TYR	CB-CA-C	5.03	118.06	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	334	GLN	CA-C-O	-5.02	115.88	121.81
2	M	313	ARG	CB-CA-C	5.02	119.65	110.11
1	C	136	ASN	O-C-N	5.02	127.44	122.12
2	R	444	PRO	CA-C-O	-5.02	115.53	122.15
1	C	197	PHE	CB-CA-C	5.01	119.21	109.33
2	Q	387	GLN	CA-C-O	-5.01	113.42	119.49
2	R	336	LEU	N-CA-C	-5.01	103.53	110.35
2	R	383	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	C	94	ARG	NE-CZ-NH1	-5.00	116.50	121.50
2	Q	429	CYS	CB-CA-C	5.00	118.63	110.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	184	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	49	0
1	B	1571	0	1499	55	0
1	C	1571	0	1499	58	0
1	D	1571	0	1499	57	0
1	E	1571	0	1499	69	0
1	F	1571	0	1499	87	0
2	M	1840	0	1794	68	0
2	N	1840	0	1794	59	0
2	O	1840	0	1794	64	0
2	P	1840	0	1794	81	0
2	Q	1840	0	1794	71	0
2	R	1840	0	1794	75	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	1	0
3	P	2	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	2	0	0	2	0
3	R	2	0	0	2	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	2	0
5	R	11	0	3	0	0
6	A	76	0	0	2	0
6	B	78	0	0	0	0
6	C	79	0	0	0	0
6	D	78	0	0	0	0
6	E	76	0	0	3	0
6	F	82	0	0	1	0
6	M	156	0	0	6	0
6	N	159	0	0	6	0
6	O	157	0	0	7	0
6	P	152	0	0	8	0
6	Q	165	0	0	8	0
6	R	152	0	0	6	0
All	All	21960	0	19776	711	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 18.

All (711) 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:134:GLY:HA3	2:N:326:THR:HG22	1.33	1.07
1:B:165:GLN:H	1:B:165:GLN:NE2	1.52	1.07
1:E:165:GLN:H	1:E:165:GLN:HE21	1.02	1.02
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.44	0.99
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.45	0.96
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.47	0.94
2:P:390:LYS:HD2	6:P:647:HOH:O	1.68	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:361:HIS:H	2:R:361:HIS:CD2	1.84	0.92
1:E:165:GLN:H	1:E:165:GLN:NE2	1.66	0.91
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.49	0.91
2:R:497:ASN:ND2	2:R:499:GLU:H	1.68	0.91
2:R:497:ASN:HD22	2:R:499:GLU:H	1.08	0.91
1:B:165:GLN:N	1:B:165:GLN:HE21	1.68	0.90
2:M:390:LYS:HD2	6:M:641:HOH:O	1.72	0.89
1:F:176:GLU:HG3	1:F:180:LYS:O	1.73	0.89
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.55	0.88
1:B:165:GLN:H	1:B:165:GLN:HE21	0.92	0.88
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.56	0.87
1:D:78:GLU:HG2	2:P:301:PRO:HG2	1.56	0.86
2:R:361:HIS:H	2:R:361:HIS:HD2	1.18	0.86
2:M:361:HIS:H	2:M:361:HIS:CD2	1.92	0.86
1:C:64:ARG:NH2	1:C:100:ASP:O	2.09	0.85
1:F:165:GLN:H	1:F:165:GLN:HE21	1.24	0.85
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.56	0.85
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.59	0.85
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.56	0.85
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.25	0.85
1:D:64:ARG:NH2	1:D:100:ASP:O	2.10	0.84
2:Q:356:PHE:CZ	2:Q:430:LEU:HD13	2.13	0.84
2:O:390:LYS:HD3	6:O:649:HOH:O	1.78	0.83
2:R:497:ASN:HD22	2:R:499:GLU:N	1.77	0.82
2:O:356:PHE:CD1	2:O:428:ARG:HD2	2.14	0.82
2:P:497:ASN:HD22	2:P:499:GLU:H	1.26	0.82
1:B:176:GLU:HG3	1:B:180:LYS:O	1.80	0.82
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.60	0.81
2:N:390:LYS:HD3	6:N:648:HOH:O	1.80	0.81
1:B:134:GLY:CA	2:N:326:THR:HG22	2.11	0.80
2:P:416:LEU:C	2:P:416:LEU:HD23	2.07	0.78
1:C:165:GLN:H	1:C:165:GLN:NE2	1.81	0.78
1:E:19:ILE:O	2:Q:426:VAL:HG21	1.84	0.78
2:M:361:HIS:H	2:M:361:HIS:HD2	1.27	0.78
1:F:19:ILE:O	2:R:426:VAL:HG21	1.83	0.78
2:N:307:ARG:HD2	6:N:659:HOH:O	1.84	0.77
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.66	0.77
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.49	0.77
1:F:41:LYS:HE3	1:F:87:ASN:O	1.85	0.77
1:E:165:GLN:HE21	1:E:165:GLN:N	1.83	0.76
2:M:497:ASN:ND2	2:M:499:GLU:H	1.83	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLN:H	1:F:165:GLN:NE2	1.82	0.76
2:R:416:LEU:C	2:R:416:LEU:HD23	2.10	0.76
2:R:306:SER:CB	2:R:530:GLN:HE21	1.98	0.76
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.15	0.76
2:O:361:HIS:H	2:O:361:HIS:CD2	2.04	0.75
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.67	0.75
1:B:176:GLU:OE2	1:B:179:GLY:O	2.05	0.75
2:M:497:ASN:HD22	2:M:499:GLU:H	1.33	0.74
2:M:416:LEU:C	2:M:416:LEU:HD23	2.11	0.74
2:R:536:GLU:HB2	6:R:1331:HOH:O	1.88	0.74
1:A:78:GLU:OE1	6:A:235:HOH:O	2.06	0.74
1:D:165:GLN:H	1:D:165:GLN:HE21	1.35	0.74
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.17	0.74
1:C:79:TYR:O	2:O:301:PRO:HB3	1.88	0.73
2:O:497:ASN:HD22	2:O:499:GLU:H	1.36	0.73
1:C:165:GLN:H	1:C:165:GLN:HE21	1.36	0.73
2:R:416:LEU:HD23	2:R:417:ALA:N	2.03	0.73
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.24	0.73
2:P:497:ASN:ND2	2:P:499:GLU:H	1.86	0.73
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.73
2:N:497:ASN:HD22	2:N:499:GLU:H	1.36	0.72
2:R:361:HIS:CD2	2:R:361:HIS:N	2.57	0.72
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.37	0.71
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.91	0.71
2:P:416:LEU:HD23	2:P:417:ALA:N	2.05	0.71
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.72	0.71
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.71	0.71
1:C:3:GLU:OE1	1:C:3:GLU:HA	1.90	0.71
1:D:165:GLN:H	1:D:165:GLN:NE2	1.89	0.71
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.07	0.71
1:C:176:GLU:HG3	1:C:180:LYS:O	1.90	0.70
2:N:416:LEU:HD23	2:N:417:ALA:N	2.06	0.70
2:O:497:ASN:ND2	2:O:499:GLU:H	1.89	0.70
2:R:356:PHE:CD2	2:R:428:ARG:HD3	2.26	0.70
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.40	0.70
1:D:78:GLU:CG	2:P:301:PRO:HG2	2.22	0.69
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.93	0.69
2:P:361:HIS:H	2:P:361:HIS:CD2	2.11	0.69
2:N:361:HIS:CD2	2:N:361:HIS:H	2.10	0.69
1:F:15:PRO:HD2	3:R:575:CYN:N	2.07	0.69
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.20	0.69
1:F:51:LEU:HD12	1:F:106:LEU:HD23	1.74	0.69
1:D:176:GLU:HG3	1:D:180:LYS:O	1.93	0.69
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.73	0.69
2:P:497:ASN:HD22	2:P:499:GLU:N	1.91	0.68
2:M:497:ASN:HD22	2:M:497:ASN:C	2.01	0.68
2:N:416:LEU:HD23	2:N:416:LEU:C	2.19	0.68
1:F:52:LEU:HD21	1:F:184:ARG:HH12	1.58	0.68
2:O:390:LYS:HE2	6:O:728:HOH:O	1.92	0.68
1:F:113:VAL:HG13	1:F:122:MET:O	1.93	0.67
2:N:488:MET:CE	1:C:1:PRO:HG3	2.24	0.67
2:Q:356:PHE:HD1	2:Q:428:ARG:HD2	1.60	0.67
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.77	0.67
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.28	0.67
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.60	0.67
1:E:134:GLY:HA3	2:Q:326:THR:CG2	2.24	0.66
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.76	0.66
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.11	0.66
2:O:356:PHE:HE1	2:O:428:ARG:HD3	1.60	0.65
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.27	0.65
2:R:306:SER:OG	2:R:530:GLN:NE2	2.28	0.65
1:A:165:GLN:H	1:A:165:GLN:NE2	1.94	0.65
2:Q:390:LYS:HD3	6:Q:1016:HOH:O	1.96	0.65
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.10	0.65
1:B:64:ARG:NH2	1:B:100:ASP:O	2.29	0.65
1:C:134:GLY:HA3	2:O:326:THR:HG22	1.79	0.65
2:M:536:GLU:HB2	6:M:697:HOH:O	1.97	0.64
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.13	0.64
2:Q:399:MET:HA	2:Q:462:HIS:O	1.98	0.64
1:B:98:THR:O	1:B:102:GLY:HA2	1.97	0.64
2:N:497:ASN:ND2	2:N:499:GLU:H	1.96	0.64
1:E:69:GLU:OE1	2:Q:473:LYS:HE2	1.98	0.64
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.28	0.64
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.78	0.64
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.22	0.64
1:C:19:ILE:O	2:O:426:VAL:HG21	1.98	0.63
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.79	0.63
2:O:497:ASN:HD22	2:O:497:ASN:C	2.07	0.63
2:R:406:GLY:O	2:R:447:TYR:HD1	1.82	0.63
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.26	0.63
2:Q:390:LYS:HE2	6:Q:1133:HOH:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.63	0.63
2:N:364:LEU:CD2	2:N:440:ARG:HD3	2.27	0.63
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.29	0.63
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.14	0.63
1:F:44:ALA:O	1:F:48:HIS:NE2	2.22	0.63
2:R:400:TRP:HA	2:R:425:GLY:O	1.99	0.63
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.81	0.63
2:M:359:HIS:O	2:M:366:ASN:HB3	1.99	0.62
1:B:176:GLU:HG3	1:B:180:LYS:C	2.25	0.62
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.80	0.62
1:C:65:ASP:OD2	1:C:133:ARG:HD3	1.99	0.62
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.15	0.62
2:R:364:LEU:HD22	2:R:440:ARG:CD	2.29	0.61
2:R:531:ARG:NH1	2:R:532:LYS:O	2.33	0.61
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.81	0.61
2:O:484:PRO:O	2:O:488:MET:HE3	2.00	0.61
2:Q:356:PHE:CD1	2:Q:428:ARG:HD2	2.35	0.61
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.46	0.61
1:F:50:LEU:HD23	1:F:182:ALA:HB2	1.82	0.61
1:F:19:ILE:HD11	2:R:408:TYR:HD1	1.65	0.61
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.15	0.61
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.01	0.61
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.49	0.61
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.35	0.61
2:R:399:MET:HA	2:R:462:HIS:O	2.01	0.61
1:B:134:GLY:HA3	2:N:326:THR:CG2	2.22	0.60
2:O:359:HIS:O	2:O:366:ASN:HB3	2.01	0.60
1:D:33:GLN:HB3	1:D:85:LEU:HD11	1.82	0.60
1:E:134:GLY:CA	2:Q:326:THR:HG22	2.25	0.60
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.02	0.60
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.36	0.60
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.48	0.60
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.37	0.60
2:N:385:VAL:O	2:N:526:VAL:HA	2.01	0.60
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.37	0.60
2:R:385:VAL:O	2:R:526:VAL:HA	2.02	0.60
2:M:326:THR:CG2	2:M:330:ARG:HD2	2.32	0.60
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.36	0.60
2:R:392:VAL:HG12	2:R:395:THR:HB	1.84	0.60
1:E:36:TRP:CG	1:E:37:ASN:H	2.20	0.60
1:A:134:GLY:HA3	2:M:326:THR:CG2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.98	0.60
1:B:3:GLU:CA	1:B:3:GLU:OE1	2.49	0.59
1:B:28:ASN:HB3	1:B:29:PRO:HD2	1.84	0.59
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.02	0.59
2:P:361:HIS:H	2:P:361:HIS:HD2	1.48	0.59
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.32	0.59
1:D:98:THR:O	1:D:102:GLY:HA2	2.03	0.59
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.65	0.59
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.02	0.59
1:E:98:THR:O	1:E:102:GLY:HA2	2.02	0.59
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.67	0.59
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.37	0.58
1:C:64:ARG:NE	1:C:100:ASP:O	2.37	0.58
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.33	0.58
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.84	0.58
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.39	0.58
1:E:113:VAL:HG23	1:E:124:PRO:HG3	1.85	0.58
2:M:376:GLU:HG2	2:P:446:PRO:HD2	1.86	0.58
2:Q:473:LYS:NZ	6:Q:1032:HOH:O	2.36	0.58
2:R:497:ASN:ND2	2:R:499:GLU:N	2.45	0.58
2:P:362:ASP:OD1	2:P:440:ARG:HD2	2.04	0.58
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.34	0.58
2:N:390:LYS:HE2	6:N:726:HOH:O	2.03	0.58
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.85	0.58
1:F:58:GLY:HA3	1:F:190:GLN:OE1	2.04	0.58
2:O:361:HIS:H	2:O:361:HIS:HD2	1.48	0.58
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.18	0.57
1:E:176:GLU:HA	1:E:180:LYS:O	2.04	0.57
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.85	0.57
2:O:416:LEU:C	2:O:416:LEU:HD23	2.29	0.57
1:F:155:CYS:O	1:F:159:ASN:ND2	2.38	0.57
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.04	0.57
1:E:15:PRO:HD2	3:Q:575:CYN:N	2.20	0.57
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.03	0.57
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.04	0.57
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.87	0.57
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.20	0.57
1:A:176:GLU:HA	1:A:180:LYS:O	2.06	0.56
2:M:416:LEU:C	2:M:416:LEU:CD2	2.77	0.56
2:Q:522:ARG:NH1	6:Q:1053:HOH:O	2.38	0.56
2:N:381:ALA:HB2	2:N:438:SER:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.35	0.56
1:C:78:GLU:CD	2:O:301:PRO:HG2	2.31	0.56
2:O:356:PHE:CE1	2:O:428:ARG:CD	2.87	0.56
1:D:78:GLU:CD	2:P:301:PRO:HG2	2.29	0.56
2:P:376:GLU:O	2:P:442:ILE:HA	2.04	0.56
2:Q:307:ARG:HD2	6:Q:1037:HOH:O	2.05	0.56
1:B:143:LEU:C	1:B:143:LEU:HD23	2.30	0.56
2:N:313:ARG:O	2:N:318:LYS:HE2	2.04	0.56
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.69	0.56
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.69	0.56
1:E:176:GLU:HG3	1:E:180:LYS:C	2.31	0.56
1:C:143:LEU:HD23	1:C:143:LEU:C	2.31	0.56
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.88	0.56
2:M:473:LYS:HD2	2:M:474:LEU:N	2.21	0.55
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.41	0.55
1:A:176:GLU:HG2	1:A:179:GLY:HA2	1.87	0.55
2:M:448:PRO:HB2	2:P:516:MET:HA	1.88	0.55
1:F:131:PHE:O	1:F:132:ALA:HB2	2.07	0.55
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.87	0.55
2:R:356:PHE:CE2	2:R:428:ARG:HD3	2.42	0.55
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.70	0.55
2:O:522:ARG:NH1	6:O:672:HOH:O	2.35	0.55
2:Q:409:ARG:HA	2:Q:419:LEU:HD21	1.87	0.55
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.87	0.55
1:D:131:PHE:CE1	1:D:138:HIS:HB3	2.41	0.55
2:R:394:ASN:HA	2:R:431:THR:O	2.06	0.55
1:D:33:GLN:HB3	1:D:85:LEU:CD1	2.36	0.55
1:D:100:ASP:OD1	1:D:100:ASP:N	2.37	0.55
1:E:1:PRO:HB2	6:E:201:HOH:O	2.07	0.55
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.55
2:M:399:MET:HA	2:M:462:HIS:O	2.07	0.55
1:C:176:GLU:HG3	1:C:180:LYS:C	2.31	0.55
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.07	0.55
1:F:50:LEU:O	1:F:182:ALA:HA	2.07	0.55
1:C:64:ARG:CZ	1:C:100:ASP:O	2.55	0.54
1:D:52:LEU:HA	1:D:104:TRP:O	2.05	0.54
1:E:161:ILE:O	1:E:167:ARG:NH2	2.34	0.54
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.37	0.54
1:F:176:GLU:HG3	1:F:180:LYS:C	2.32	0.54
1:C:100:ASP:OD1	1:C:100:ASP:N	2.40	0.54
2:R:395:THR:HG22	2:R:431:THR:CG2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.42	0.54
2:R:478:LEU:C	2:R:478:LEU:HD23	2.33	0.54
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.08	0.54
2:M:314:ASN:OD1	2:M:318:LYS:HE2	2.07	0.54
2:M:356:PHE:HE1	2:M:428:ARG:HD2	1.73	0.54
1:C:16:TYR:O	1:C:19:ILE:HG23	2.08	0.54
1:E:67:PHE:C	1:E:68:LEU:HD12	2.31	0.54
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.43	0.54
2:M:326:THR:HG22	2:M:326:THR:O	2.07	0.54
2:N:361:HIS:H	2:N:361:HIS:HD2	1.55	0.54
2:Q:356:PHE:CE2	2:Q:430:LEU:HD13	2.43	0.54
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.43	0.54
2:N:359:HIS:O	2:N:366:ASN:HB3	2.08	0.54
1:C:36:TRP:CG	1:C:37:ASN:H	2.26	0.54
1:F:92:PHE:CG	2:R:349:PRO:HG3	2.43	0.54
1:A:79:TYR:O	2:M:301:PRO:HB2	2.08	0.54
1:D:134:GLY:HA3	2:P:326:THR:CG2	2.34	0.54
1:D:66:SER:HA	1:D:132:ALA:HB2	1.89	0.53
1:E:68:LEU:HD12	1:E:68:LEU:N	2.22	0.53
1:A:78:GLU:CG	2:M:301:PRO:HG3	2.39	0.53
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.73	0.53
3:R:575:CYN:C	6:R:1181:HOH:O	2.56	0.53
2:P:319:ALA:HB3	6:P:684:HOH:O	2.08	0.53
1:E:143:LEU:HD23	1:E:143:LEU:C	2.33	0.53
1:F:19:ILE:O	2:R:426:VAL:CG2	2.56	0.53
1:A:28:ASN:HB3	6:A:265:HOH:O	2.08	0.53
1:A:100:ASP:OD1	1:A:100:ASP:N	2.38	0.53
2:P:362:ASP:OD1	2:P:364:LEU:HB2	2.08	0.53
1:E:176:GLU:HG3	1:E:180:LYS:O	2.09	0.53
2:O:505:ILE:HG22	2:O:507:LYS:CE	2.38	0.53
1:D:191:GLY:O	1:D:194:GLU:HB2	2.09	0.53
1:E:24:GLU:O	1:E:27:GLY:N	2.41	0.53
2:Q:364:LEU:CD2	2:Q:440:ARG:HD3	2.38	0.53
1:D:51:LEU:O	1:D:105:THR:HA	2.08	0.53
2:R:484:PRO:O	2:R:488:MET:HE3	2.08	0.53
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.24	0.53
1:E:100:ASP:OD1	1:E:100:ASP:N	2.42	0.53
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.06	0.53
1:C:3:GLU:OE1	1:C:3:GLU:CA	2.51	0.52
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.91	0.52
1:E:41:LYS:HD2	1:E:87:ASN:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TRP:CG	1:D:37:ASN:H	2.27	0.52
1:E:52:LEU:HD23	1:E:184:ARG:NH1	2.24	0.52
1:E:92:PHE:CG	2:Q:349:PRO:HG3	2.44	0.52
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.91	0.52
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.39	0.52
1:B:19:ILE:CG2	2:N:410:HIS:HB2	2.40	0.52
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.91	0.52
2:R:405:GLY:HA3	6:R:1255:HOH:O	2.08	0.52
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.44	0.52
2:P:416:LEU:C	2:P:416:LEU:CD2	2.80	0.52
1:E:92:PHE:CD1	2:Q:349:PRO:HG3	2.45	0.52
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.10	0.52
1:A:36:TRP:CG	1:A:37:ASN:H	2.27	0.52
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.52
1:B:4:LEU:HD22	2:P:511:ASN:OD1	2.09	0.52
1:C:71:TRP:CD1	2:O:470:ILE:HD13	2.45	0.52
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.42	0.52
2:N:497:ASN:HD22	2:N:497:ASN:C	2.16	0.52
1:C:64:ARG:HH21	1:C:100:ASP:C	2.16	0.52
2:O:478:LEU:HD23	2:O:478:LEU:C	2.34	0.52
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.25	0.51
1:D:134:GLY:CA	2:P:326:THR:HG22	2.35	0.51
2:N:363:LEU:HD11	2:N:427:GLY:HA3	1.92	0.51
1:D:131:PHE:CD1	1:D:138:HIS:HB3	2.45	0.51
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.10	0.51
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.44	0.51
2:R:497:ASN:HD22	2:R:497:ASN:C	2.18	0.51
2:M:356:PHE:CE1	2:M:428:ARG:HD2	2.45	0.51
1:C:50:LEU:HD12	1:C:51:LEU:N	2.25	0.51
2:O:497:ASN:HD22	2:O:498:PRO:N	2.07	0.51
2:P:359:HIS:O	2:P:366:ASN:HB3	2.11	0.51
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	1.92	0.51
2:P:478:LEU:C	2:P:478:LEU:HD23	2.35	0.51
1:E:115:ASN:HA	1:E:121:PRO:HA	1.93	0.51
1:F:35:ILE:CG2	1:F:94:ARG:HG3	2.36	0.51
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.93	0.51
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.10	0.51
1:C:176:GLU:HA	1:C:180:LYS:O	2.10	0.51
2:M:405:GLY:HA3	6:M:644:HOH:O	2.11	0.51
2:P:497:ASN:HD22	2:P:497:ASN:C	2.18	0.51
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:LEU:CD2	1:F:184:ARG:HH12	2.24	0.51
2:M:390:LYS:HD3	6:M:719:HOH:O	2.10	0.51
1:F:50:LEU:HD23	1:F:182:ALA:CB	2.41	0.51
2:M:363:LEU:N	2:M:363:LEU:HD12	2.25	0.51
2:P:362:ASP:OD2	2:P:440:ARG:NH1	2.44	0.50
1:C:15:PRO:HD2	3:O:575:CYN:N	2.27	0.50
2:P:405:GLY:HA3	6:P:650:HOH:O	2.11	0.50
2:P:434:ASP:HB3	2:P:436:TYR:HD2	1.74	0.50
2:M:328:ILE:HD12	2:N:335:ALA:HB2	1.92	0.50
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.50
2:O:307:ARG:HD2	6:O:661:HOH:O	2.11	0.50
2:P:305:ASN:N	6:P:733:HOH:O	2.39	0.50
1:F:174:ARG:HE	1:F:181:THR:HG23	1.75	0.50
1:A:1:PRO:HG2	2:O:488:MET:HE2	1.94	0.50
1:A:66:SER:HB2	1:A:130:LEU:HD11	1.92	0.50
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.12	0.50
2:O:505:ILE:HG22	2:O:507:LYS:HE2	1.92	0.50
2:P:536:GLU:HB2	6:P:701:HOH:O	2.11	0.50
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.94	0.50
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.94	0.50
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.45	0.50
2:N:536:GLU:HB2	6:N:702:HOH:O	2.10	0.50
1:E:5:LEU:HG	6:Q:1093:HOH:O	2.11	0.50
1:B:98:THR:HB	1:B:100:ASP:OD1	2.11	0.50
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.93	0.50
2:Q:364:LEU:HD22	2:Q:440:ARG:CG	2.42	0.50
1:B:133:ARG:HG2	2:N:326:THR:HG21	1.93	0.50
1:D:143:LEU:C	1:D:143:LEU:HD23	2.35	0.50
2:P:533:THR:HA	6:P:632:HOH:O	2.12	0.50
1:E:177:VAL:HG12	1:E:178:ASP:OD2	2.12	0.50
1:F:143:LEU:C	1:F:143:LEU:HD23	2.36	0.50
2:R:356:PHE:HD2	2:R:428:ARG:HD3	1.75	0.50
2:M:324:TYR:OH	5:M:550:INO:O1	2.25	0.50
1:B:36:TRP:CG	1:B:37:ASN:H	2.29	0.50
1:F:48:HIS:HA	1:F:109:VAL:HG12	1.94	0.50
1:B:176:GLU:OE2	1:B:179:GLY:C	2.54	0.49
2:N:488:MET:HE2	1:C:1:PRO:HG3	1.93	0.49
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.92	0.49
2:R:416:LEU:C	2:R:416:LEU:CD2	2.83	0.49
1:A:165:GLN:H	1:A:165:GLN:CD	2.20	0.49
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.41	0.49
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.43	0.49
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.95	0.49
1:E:18:HIS:CE1	1:E:99:PHE:CE1	3.01	0.49
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.47	0.49
2:R:306:SER:HB3	2:R:530:GLN:HG3	1.94	0.49
1:A:52:LEU:C	1:A:52:LEU:HD22	2.37	0.49
2:O:505:ILE:O	2:O:507:LYS:HE3	2.11	0.49
2:R:359:HIS:O	2:R:366:ASN:HB3	2.12	0.49
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.47	0.49
1:F:19:ILE:HD11	2:R:408:TYR:CD1	2.47	0.49
1:F:78:GLU:HB2	1:F:80:GLN:HE21	1.77	0.49
2:M:406:GLY:O	2:M:447:TYR:HD1	1.95	0.49
2:R:383:ARG:HA	2:R:435:GLY:O	2.13	0.49
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.60	0.49
1:F:78:GLU:HB2	1:F:80:GLN:NE2	2.28	0.49
2:R:350:ASN:OD1	2:R:350:ASN:C	2.55	0.49
2:N:392:VAL:HG12	2:N:395:THR:HB	1.95	0.49
1:C:80:GLN:HA	1:C:80:GLN:OE1	2.13	0.49
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.75	0.49
1:F:36:TRP:HA	1:F:36:TRP:CE3	2.46	0.49
2:M:522:ARG:NH1	6:M:665:HOH:O	2.44	0.48
1:D:176:GLU:HA	1:D:180:LYS:O	2.13	0.48
1:E:18:HIS:CE1	1:E:99:PHE:HE1	2.31	0.48
2:R:536:GLU:HG3	6:R:1224:HOH:O	2.11	0.48
1:B:52:LEU:CD2	1:B:184:ARG:NH1	2.76	0.48
1:D:15:PRO:HD2	3:P:575:CYN:N	2.28	0.48
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.73	0.48
1:F:115:ASN:HA	1:F:121:PRO:HA	1.94	0.48
1:C:98:THR:O	1:C:102:GLY:HA2	2.13	0.48
1:E:41:LYS:HZ1	1:E:86:GLU:HA	1.78	0.48
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.79	0.48
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.94	0.48
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.96	0.48
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.48	0.48
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.43	0.48
1:F:74:ASP:OD1	1:F:74:ASP:C	2.54	0.48
1:C:78:GLU:CG	2:O:301:PRO:HG2	2.44	0.48
2:Q:356:PHE:HZ	2:Q:430:LEU:HD13	1.70	0.48
1:F:154:LYS:HD2	1:F:154:LYS:HA	1.55	0.48
1:B:165:GLN:NE2	1:B:165:GLN:N	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:386:ASP:HA	2:N:527:LEU:O	2.13	0.47
2:P:497:ASN:HD21	2:P:499:GLU:HB2	1.76	0.47
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.96	0.47
1:F:18:HIS:CE1	1:F:99:PHE:CE1	3.02	0.47
2:M:468:PRO:HD2	2:M:472:THR:HG21	1.96	0.47
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.22	0.47
2:M:403:ASN:OD1	2:M:403:ASN:C	2.56	0.47
2:N:376:GLU:O	2:N:442:ILE:HA	2.14	0.47
2:Q:350:ASN:C	2:Q:350:ASN:OD1	2.57	0.47
1:F:52:LEU:C	1:F:52:LEU:HD22	2.40	0.47
1:F:74:ASP:OD1	1:F:76:ASN:N	2.48	0.47
1:F:77:GLY:O	1:F:114:VAL:HG12	2.15	0.47
1:A:51:LEU:HD11	1:A:126:ILE:HD12	1.97	0.47
1:A:114:VAL:HG23	1:A:122:MET:CE	2.43	0.47
2:M:497:ASN:HD22	2:M:498:PRO:N	2.11	0.47
1:D:50:LEU:O	1:D:182:ALA:HA	2.14	0.47
2:Q:447:TYR:CE2	5:Q:550:INO:H6	2.48	0.47
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.82	0.47
1:F:39:LEU:N	1:F:39:LEU:HD12	2.29	0.47
2:R:387:GLN:HG3	2:R:527:LEU:O	2.14	0.47
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.61	0.47
2:M:326:THR:CG2	2:M:326:THR:O	2.62	0.47
2:O:395:THR:HG22	2:O:431:THR:CG2	2.44	0.47
1:E:52:LEU:C	1:E:52:LEU:HD22	2.39	0.47
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.37	0.47
2:R:392:VAL:HG21	2:R:527:LEU:HD12	1.95	0.47
1:D:63:VAL:HG13	2:P:330:ARG:CZ	2.45	0.47
1:D:64:ARG:CZ	1:D:100:ASP:O	2.63	0.47
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.97	0.47
2:P:304:ASP:CG	2:P:307:ARG:HH12	2.22	0.47
2:O:392:VAL:HG12	2:O:395:THR:HB	1.96	0.47
2:O:406:GLY:O	2:O:447:TYR:HD1	1.98	0.47
2:P:385:VAL:O	2:P:526:VAL:HA	2.15	0.47
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.33	0.47
2:M:516:MET:HA	2:P:448:PRO:HB2	1.96	0.46
1:C:116:ASN:C	1:C:116:ASN:OD1	2.58	0.46
1:D:79:TYR:O	2:P:301:PRO:HB3	2.15	0.46
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.79	0.46
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.98	0.46
1:B:12:THR:HA	1:B:135:ILE:O	2.16	0.46
1:E:13:ALA:HB2	2:Q:475:ILE:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASP:HB3	1:B:171:ILE:HG22	1.97	0.46
2:O:405:GLY:HA3	6:O:652:HOH:O	2.15	0.46
2:M:515:PRO:HB3	2:P:453:PRO:O	2.16	0.46
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.98	0.46
2:N:399:MET:HA	2:N:462:HIS:O	2.15	0.46
2:N:486:ILE:N	2:N:487:PRO:HD2	2.30	0.46
2:O:395:THR:HG22	2:O:431:THR:HG23	1.98	0.46
1:E:66:SER:HB2	1:E:130:LEU:HD11	1.98	0.46
2:M:361:HIS:CD2	2:M:361:HIS:N	2.64	0.46
2:O:434:ASP:HB3	2:O:436:TYR:CE2	2.51	0.46
1:E:31:ARG:O	1:E:32:ASP:C	2.59	0.46
1:F:124:PRO:HA	6:F:1221:HOH:O	2.15	0.46
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.96	0.46
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.51	0.46
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.51	0.46
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.87	0.46
2:M:497:ASN:ND2	2:M:499:GLU:N	2.59	0.46
1:E:51:LEU:HD12	1:E:106:LEU:CD2	2.46	0.46
2:M:486:ILE:N	2:M:487:PRO:CD	2.78	0.46
1:E:180:LYS:HG2	1:E:181:THR:N	2.30	0.46
1:F:31:ARG:HB3	6:R:1327:HOH:O	2.16	0.46
1:A:199:ASP:CG	2:M:313:ARG:HE	2.24	0.45
1:C:98:THR:OG1	1:C:102:GLY:N	2.49	0.45
1:F:36:TRP:CG	1:F:37:ASN:H	2.34	0.45
1:F:125:HIS:HA	1:F:143:LEU:O	2.16	0.45
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.97	0.45
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.45
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.30	0.45
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.16	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.77	0.45
1:C:39:LEU:HD11	1:C:93:GLY:HA3	1.97	0.45
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.97	0.45
2:N:465:ILE:HD13	2:N:525:ILE:HG21	1.97	0.45
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.97	0.45
2:O:395:THR:O	2:O:430:LEU:HA	2.17	0.45
2:P:406:GLY:O	2:P:447:TYR:HD1	1.98	0.45
2:P:473:LYS:HD3	6:P:715:HOH:O	2.16	0.45
1:F:54:GLN:HG3	1:F:184:ARG:HH21	1.82	0.45
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.15	0.45
1:F:150:GLN:O	1:F:153:ALA:HB3	2.16	0.45
2:R:395:THR:HG22	2:R:431:THR:HG23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.16	0.45
1:F:35:ILE:HG21	1:F:92:PHE:CE2	2.52	0.45
1:B:115:ASN:HA	1:B:121:PRO:HA	1.97	0.45
1:E:87:ASN:HB3	1:E:89:PHE:O	2.17	0.45
1:F:44:ALA:HA	1:F:45:PRO:HD2	1.81	0.45
1:B:31:ARG:HD2	2:N:428:ARG:NH2	2.32	0.45
1:C:52:LEU:C	1:C:52:LEU:HD22	2.41	0.45
1:D:19:ILE:HG22	1:D:26:ALA:HB1	1.98	0.45
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.11	0.45
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.99	0.45
1:B:199:ASP:CG	2:N:313:ARG:HE	2.25	0.45
2:O:326:THR:HG22	2:O:326:THR:O	2.16	0.45
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.98	0.45
1:E:110:LYS:HG3	1:E:111:PRO:HD2	1.99	0.45
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.47	0.45
2:Q:404:ALA:HB2	2:Q:442:ILE:HD13	1.99	0.45
1:A:50:LEU:O	1:A:182:ALA:HA	2.17	0.45
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.83	0.45
1:A:176:GLU:HG3	1:A:180:LYS:O	2.17	0.45
2:Q:415:TYR:CE1	2:Q:416:LEU:CD2	3.00	0.45
2:R:495:ILE:HG21	2:R:500:ALA:HB3	1.99	0.45
1:B:50:LEU:O	1:B:182:ALA:HA	2.17	0.45
2:N:511:ASN:OD1	6:N:742:HOH:O	2.21	0.45
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.99	0.44
2:P:304:ASP:OD1	2:P:307:ARG:NH1	2.48	0.44
1:A:24:GLU:O	1:A:27:GLY:N	2.46	0.44
2:O:306:SER:CB	2:O:530:GLN:HE21	2.30	0.44
2:O:381:ALA:O	2:O:522:ARG:HA	2.17	0.44
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.52	0.44
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.99	0.44
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.66	0.44
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.99	0.44
1:E:51:LEU:HD11	1:E:126:ILE:HD12	1.98	0.44
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.62	0.44
2:P:400:TRP:HA	2:P:425:GLY:O	2.17	0.44
1:F:33:GLN:HB3	1:F:85:LEU:HD11	1.99	0.44
1:F:41:LYS:O	1:F:44:ALA:N	2.50	0.44
1:F:110:LYS:NZ	1:F:147:ASP:OD1	2.35	0.44
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.81	0.44
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.48	0.44
1:B:23:LEU:HD12	1:B:23:LEU:H	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.32	0.44
2:P:410:HIS:ND1	2:P:411:LYS:N	2.66	0.44
1:E:52:LEU:CD2	1:E:184:ARG:HH11	2.30	0.44
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.32	0.44
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.99	0.44
1:D:150:GLN:O	1:D:154:LYS:HG2	2.18	0.44
2:Q:447:TYR:CD2	5:Q:550:INO:H6	2.53	0.44
2:M:488:MET:CE	2:P:508:LEU:HD23	2.48	0.44
2:N:490:PRO:HA	2:N:493:LYS:HE2	2.00	0.44
2:P:364:LEU:HB2	2:P:440:ARG:HD3	2.00	0.44
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.73	0.44
2:Q:449:TRP:CD1	2:Q:449:TRP:N	2.85	0.44
1:F:48:HIS:CD2	1:F:48:HIS:N	2.85	0.44
2:M:508:LEU:HD23	2:P:488:MET:CE	2.44	0.44
2:O:489:CYS:C	2:O:493:LYS:HE2	2.43	0.44
1:B:52:LEU:HD23	1:B:103:GLU:CD	2.43	0.43
2:N:493:LYS:HE2	2:N:493:LYS:HB2	1.83	0.43
2:R:306:SER:O	2:R:307:ARG:NH1	2.52	0.43
1:D:64:ARG:NE	1:D:100:ASP:O	2.50	0.43
1:D:176:GLU:HG3	1:D:180:LYS:C	2.41	0.43
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.53	0.43
2:O:376:GLU:O	2:O:442:ILE:HA	2.17	0.43
1:E:38:ARG:HG3	1:E:107:HIS:HB2	2.00	0.43
2:O:415:TYR:CE1	2:O:416:LEU:HD22	2.53	0.43
1:E:32:ASP:HB2	6:E:265:HOH:O	2.17	0.43
2:Q:536:GLU:HB2	6:Q:1096:HOH:O	2.18	0.43
1:B:92:PHE:CG	2:N:349:PRO:HG3	2.53	0.43
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.34	0.43
1:D:19:ILE:O	2:P:426:VAL:HG21	2.18	0.43
2:P:373:PRO:HB3	2:P:423:PHE:HB2	2.00	0.43
2:Q:403:ASN:HB2	6:Q:960:HOH:O	2.19	0.43
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.54	0.43
1:B:176:GLU:HA	1:B:180:LYS:O	2.19	0.43
2:O:308:PHE:CE2	2:O:530:GLN:HB2	2.52	0.43
2:O:399:MET:HA	2:O:462:HIS:O	2.18	0.43
1:D:19:ILE:CG2	2:P:410:HIS:HB2	2.48	0.43
1:E:54:GLN:OE1	1:E:184:ARG:NH2	2.52	0.43
2:R:307:ARG:CG	2:R:533:THR:HG22	2.49	0.43
2:M:450:ARG:HG3	6:M:632:HOH:O	2.19	0.43
1:B:2:ILE:O	1:B:3:GLU:OE1	2.37	0.43
2:P:315:TRP:CZ2	2:P:503:GLN:NE2	2.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:404:ALA:HB2	2:P:442:ILE:HD12	2.01	0.43
2:M:385:VAL:O	2:M:526:VAL:HA	2.17	0.43
2:M:488:MET:HE1	2:P:508:LEU:HD23	2.00	0.43
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.54	0.43
1:B:52:LEU:HD21	1:B:184:ARG:HH12	1.84	0.43
1:C:12:THR:HA	1:C:135:ILE:O	2.19	0.43
1:C:36:TRP:HA	1:C:36:TRP:CE3	2.53	0.43
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.54	0.43
2:Q:363:LEU:HD11	2:Q:427:GLY:HA3	1.99	0.43
2:M:437:TYR:CD1	2:M:437:TYR:C	2.96	0.42
2:Q:362:ASP:OD1	2:Q:364:LEU:HB2	2.19	0.42
2:Q:395:THR:HG22	2:Q:431:THR:HG23	2.01	0.42
2:Q:493:LYS:HE3	2:Q:493:LYS:HB2	1.67	0.42
1:F:143:LEU:HD23	1:F:144:TYR:N	2.34	0.42
1:A:157:VAL:O	1:A:160:LEU:HB2	2.19	0.42
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.89	0.42
2:O:460:HIS:HB3	2:O:479:TYR:CD1	2.54	0.42
1:D:26:ALA:O	2:P:411:LYS:HG3	2.18	0.42
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.84	0.42
6:E:204:HOH:O	3:Q:575:CYN:C	2.66	0.42
1:F:54:GLN:HG3	1:F:184:ARG:NH2	2.33	0.42
1:F:64:ARG:HD3	1:F:99:PHE:O	2.19	0.42
1:A:12:THR:HA	1:A:135:ILE:O	2.19	0.42
2:M:519:LEU:HA	2:M:519:LEU:HD23	1.85	0.42
2:N:363:LEU:HD12	2:N:363:LEU:N	2.34	0.42
2:Q:509:ASP:N	2:Q:520:ALA:O	2.41	0.42
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.54	0.42
2:R:434:ASP:HB3	2:R:436:TYR:HD2	1.82	0.42
1:A:114:VAL:CG2	1:A:122:MET:HE3	2.49	0.42
2:O:437:TYR:CD1	2:O:437:TYR:C	2.97	0.42
1:D:39:LEU:HD12	1:D:39:LEU:N	2.34	0.42
1:D:165:GLN:HE21	1:D:165:GLN:N	2.11	0.42
1:F:8:THR:HA	1:F:9:PRO:HD3	1.86	0.42
2:R:437:TYR:CD2	2:R:437:TYR:C	2.96	0.42
2:R:472:THR:O	2:R:473:LYS:C	2.62	0.42
1:B:63:VAL:HG13	2:N:330:ARG:CZ	2.50	0.42
1:B:176:GLU:HG2	1:B:179:GLY:C	2.44	0.42
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.75	0.42
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.84	0.42
1:D:39:LEU:HB3	1:D:90:ASN:O	2.20	0.42
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:THR:OG1	1:E:109:VAL:N	2.49	0.42
1:F:40:ALA:HB2	1:F:89:PHE:HD2	1.84	0.42
2:R:465:ILE:N	2:R:465:ILE:HD12	2.34	0.42
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.05	0.42
2:O:364:LEU:HD22	2:O:440:ARG:CG	2.49	0.42
1:F:32:ASP:HB2	6:R:1378:HOH:O	2.19	0.42
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.87	0.42
1:A:63:VAL:HG13	2:M:330:ARG:CZ	2.50	0.42
1:B:33:GLN:HG2	1:B:85:LEU:HD12	2.01	0.42
1:C:15:PRO:HB3	1:C:133:ARG:HD2	2.01	0.42
2:O:473:LYS:NZ	6:O:718:HOH:O	2.42	0.42
1:B:64:ARG:HH11	1:B:64:ARG:HD2	1.52	0.42
2:N:350:ASN:OD1	2:N:350:ASN:C	2.63	0.42
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.85	0.42
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.71	0.42
2:P:394:ASN:HA	2:P:431:THR:O	2.20	0.42
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	2.01	0.42
1:E:74:ASP:N	1:E:78:GLU:O	2.41	0.42
2:R:484:PRO:O	2:R:487:PRO:HD2	2.20	0.42
2:O:536:GLU:HB2	6:O:704:HOH:O	2.18	0.41
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.84	0.41
1:E:19:ILE:CG2	2:Q:410:HIS:HB2	2.50	0.41
1:E:170:LEU:HD21	1:E:196:VAL:HB	2.01	0.41
1:F:25:ALA:O	2:R:411:LYS:NZ	2.52	0.41
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.55	0.41
2:M:361:HIS:HB3	2:M:429:CYS:HB3	2.00	0.41
2:M:448:PRO:CB	2:P:516:MET:HA	2.50	0.41
2:N:364:LEU:HB2	2:N:440:ARG:HD3	2.01	0.41
2:P:381:ALA:HB2	2:P:438:SER:HB2	2.02	0.41
2:Q:487:PRO:O	2:Q:493:LYS:HD3	2.20	0.41
1:A:66:SER:HA	1:A:132:ALA:HB2	2.02	0.41
1:C:26:ALA:O	2:O:411:LYS:HG3	2.20	0.41
1:C:50:LEU:HD12	1:C:51:LEU:H	1.85	0.41
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.51	0.41
1:F:81:ASP:HB2	2:R:348:GLY:O	2.21	0.41
2:R:384:VAL:N	2:R:435:GLY:O	2.38	0.41
1:C:126:ILE:HD12	1:C:143:LEU:HD22	2.01	0.41
2:Q:306:SER:HG	2:Q:530:GLN:HE21	1.65	0.41
2:M:516:MET:HE3	2:M:516:MET:HB3	1.80	0.41
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.02	0.41
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:O	1:A:102:GLY:HA2	2.21	0.41
1:C:19:ILE:HG13	2:O:426:VAL:HG22	2.02	0.41
1:E:39:LEU:O	1:E:89:PHE:HA	2.21	0.41
1:F:33:GLN:HG2	1:F:85:LEU:CD1	2.49	0.41
1:C:52:LEU:HA	1:C:104:TRP:O	2.20	0.41
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.21	0.41
2:R:321:THR:HG21	2:R:494:SER:HB2	2.01	0.41
2:R:534:HIS:C	2:R:536:GLU:N	2.79	0.41
1:D:176:GLU:HG3	1:D:180:LYS:N	2.36	0.41
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.88	0.41
2:P:437:TYR:CD1	2:P:437:TYR:C	2.99	0.41
1:E:51:LEU:HB2	1:E:106:LEU:HB3	2.02	0.41
1:F:100:ASP:OD1	1:F:100:ASP:N	2.54	0.41
1:F:200:PHE:CG	2:R:345:GLU:HG2	2.56	0.41
1:A:9:PRO:HG3	2:M:500:ALA:HB1	2.02	0.41
1:A:78:GLU:HG2	2:M:301:PRO:HG3	2.02	0.41
1:A:180:LYS:HG2	1:A:181:THR:N	2.34	0.41
2:N:371:GLY:HA3	2:N:422:ASN:ND2	2.35	0.41
1:C:18:HIS:CE1	1:C:99:PHE:HE1	2.39	0.41
1:E:15:PRO:HB3	1:E:133:ARG:HD2	2.03	0.41
1:E:36:TRP:CD1	1:E:37:ASN:H	2.38	0.41
1:E:51:LEU:O	1:E:105:THR:HA	2.20	0.41
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.46	0.41
1:A:191:GLY:O	1:A:194:GLU:HB2	2.20	0.41
1:C:19:ILE:CG1	2:O:400:TRP:HB2	2.51	0.41
1:D:131:PHE:O	1:D:132:ALA:HB2	2.21	0.41
2:P:335:ALA:HB1	2:R:325:LYS:HD3	2.03	0.41
2:P:489:CYS:O	2:P:493:LYS:HE3	2.21	0.41
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.22	0.40
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.74	0.40
1:B:31:ARG:HB3	6:N:699:HOH:O	2.21	0.40
1:D:65:ASP:OD2	1:D:133:ARG:CD	2.68	0.40
2:P:311:ARG:HH11	2:P:311:ARG:HD2	1.68	0.40
2:P:362:ASP:CG	2:P:440:ARG:HD2	2.45	0.40
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.21	0.40
2:N:497:ASN:HD22	2:N:499:GLU:N	2.11	0.40
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.71	0.40
2:P:484:PRO:O	2:P:487:PRO:HD2	2.20	0.40
2:P:522:ARG:NH1	6:P:670:HOH:O	2.48	0.40
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.54	0.40
2:M:409:ARG:NH2	2:M:420:ASP:O	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:395:THR:O	2:Q:430:LEU:HA	2.20	0.40
2:N:307:ARG:HA	2:N:307:ARG:HD3	1.83	0.40
2:O:307:ARG:HA	2:O:307:ARG:HD3	1.94	0.40
1:D:51:LEU:HD12	1:D:106:LEU:HD23	2.03	0.40
1:D:131:PHE:CE1	1:D:138:HIS:CB	3.04	0.40
2:P:519:LEU:HD23	2:P:519:LEU:HA	1.92	0.40
2:R:395:THR:HG22	2:R:431:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	B	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	C	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	20
1	D	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	24	20
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	20
2	M	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	N	229/238 (96%)	221 (96%)	7 (3%)	1 (0%)	30	26
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	30	26
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	10 (4%)	1 (0%)	30	26
All	All	2562/2628 (98%)	2444 (95%)	112 (4%)	6 (0%)	43	44

All (6) Ramachandran outliers are listed below:

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

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	15
1	B	162/163 (99%)	151 (93%)	11 (7%)	14	10
1	C	162/163 (99%)	157 (97%)	5 (3%)	35	37
1	D	162/163 (99%)	152 (94%)	10 (6%)	16	12
1	E	162/163 (99%)	156 (96%)	6 (4%)	30	30
1	F	162/163 (99%)	152 (94%)	10 (6%)	16	12
2	M	196/202 (97%)	188 (96%)	8 (4%)	27	26
2	N	196/202 (97%)	192 (98%)	4 (2%)	48	54
2	O	196/202 (97%)	183 (93%)	13 (7%)	15	10
2	P	196/202 (97%)	187 (95%)	9 (5%)	24	22
2	Q	196/202 (97%)	179 (91%)	17 (9%)	9	5
2	R	196/202 (97%)	181 (92%)	15 (8%)	12	7
All	All	2148/2190 (98%)	2031 (95%)	117 (5%)	20	16

All (117) 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	52	LEU
1	A	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	ASP
1	A	114	VAL
1	A	165	GLN
1	A	184	ARG
2	M	343	ILE
2	M	364	LEU
2	M	395	THR
2	M	416	LEU
2	M	434	ASP
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	32	ASP
1	B	38	ARG
1	B	50	LEU
1	B	52	LEU
1	B	91	SER
1	B	109	VAL
1	B	114	VAL
1	B	133	ARG
1	B	165	GLN
1	B	176	GLU
2	N	326	THR
2	N	364	LEU
2	N	395	THR
2	N	416	LEU
1	C	4	LEU
1	C	19	ILE
1	C	52	LEU
1	C	158	LEU
1	C	165	GLN
2	O	372	LEU
2	O	395	THR
2	O	411	LYS
2	O	414	ARG
2	O	416	LEU
2	O	428	ARG
2	O	429	CYS
2	O	434	ASP
2	O	438	SER
2	O	440	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	507	LYS
2	O	511	ASN
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	43	ASP
1	D	52	LEU
1	D	78	GLU
1	D	100	ASP
1	D	109	VAL
1	D	114	VAL
1	D	165	GLN
1	D	184	ARG
2	P	364	LEU
2	P	395	THR
2	P	416	LEU
2	P	429	CYS
2	P	434	ASP
2	P	438	SER
2	P	440	ARG
2	P	450	ARG
2	P	497	ASN
1	E	19	ILE
1	E	24	GLU
1	E	52	LEU
1	E	100	ASP
1	E	165	GLN
1	E	181	THR
2	Q	326	THR
2	Q	343	ILE
2	Q	364	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	429	CYS
2	Q	430	LEU
2	Q	434	ASP
2	Q	442	ILE
2	Q	473	LYS
2	Q	478	LEU
2	Q	491	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	497	ASN
2	Q	503	GLN
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	42	PRO
1	F	50	LEU
1	F	52	LEU
1	F	68	LEU
1	F	94	ARG
1	F	100	ASP
1	F	126	ILE
1	F	165	GLN
2	R	306	SER
2	R	343	ILE
2	R	372	LEU
2	R	394	ASN
2	R	395	THR
2	R	399	MET
2	R	411	LYS
2	R	416	LEU
2	R	428	ARG
2	R	429	CYS
2	R	434	ASP
2	R	440	ARG
2	R	442	ILE
2	R	465	ILE
2	R	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	116	ASN
1	A	163	GLN
1	A	165	GLN
2	M	359	HIS
2	M	361	HIS
2	M	412	ASN
2	M	422	ASN
2	M	497	ASN
2	M	503	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	127	ASN
1	B	140	HIS
1	B	163	GLN
1	B	165	GLN
2	N	359	HIS
2	N	361	HIS
2	N	412	ASN
2	N	422	ASN
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	18	HIS
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	80	GLN
1	D	127	ASN
1	D	140	HIS
1	D	163	GLN
1	D	165	GLN
2	P	305	ASN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	502	GLN
2	P	503	GLN
2	P	530	GLN
2	P	534	HIS
1	E	127	ASN
1	E	163	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	422	ASN
2	Q	497	ASN
2	Q	530	GLN
2	Q	534	HIS
1	F	11	GLN
1	F	18	HIS
1	F	140	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	165	GLN
2	R	361	HIS
2	R	497	ASN
2	R	530	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	M	575	4	1,1,1	0.44	0	-		
3	CYN	N	575	4	1,1,1	0.42	0	-		
5	INO	M	550	4	10,11,11	2.05	4 (40%)	10,15,15	0.96	0
3	CYN	P	575	4	1,1,1	0.60	0	-		
5	INO	O	550	4	10,11,11	1.92	5 (50%)	10,15,15	1.39	2 (20%)
5	INO	N	550	4	10,11,11	1.94	4 (40%)	10,15,15	1.53	2 (20%)
5	INO	P	550	4	10,11,11	1.72	4 (40%)	10,15,15	1.21	2 (20%)
3	CYN	R	575	4	1,1,1	0.37	0	-		
3	CYN	Q	575	4	1,1,1	0.46	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	INO	R	550	4	10,11,11	1.68	4 (40%)	10,15,15	1.24	2 (20%)
3	CYN	O	575	4	1,1,1	0.29	0	-		
5	INO	Q	550	4	10,11,11	1.68	3 (30%)	10,15,15	1.40	2 (20%)

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	INO	O	550	4	-	0/4/4/4	0/1/1/1
5	INO	M	550	4	-	0/4/4/4	0/1/1/1
5	INO	N	550	4	-	0/4/4/4	0/1/1/1
5	INO	P	550	4	-	0/4/4/4	0/1/1/1
5	INO	R	550	4	-	0/4/4/4	0/1/1/1
5	INO	Q	550	4	-	0/4/4/4	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	INO	O4-N1	-3.84	1.29	1.37
5	O	550	INO	O4-N1	-3.51	1.30	1.37
5	M	550	INO	O3-C2	-3.32	1.23	1.32
5	M	550	INO	O4-N1	-3.13	1.31	1.37
5	M	550	INO	C4-C7	2.86	1.55	1.49
5	N	550	INO	O3-C2	-2.78	1.25	1.32
5	O	550	INO	O3-C2	-2.69	1.25	1.32
5	Q	550	INO	O3-C2	-2.69	1.25	1.32
5	M	550	INO	O2-C7	-2.61	1.22	1.30
5	P	550	INO	O3-C2	-2.60	1.25	1.32
5	P	550	INO	C4-C7	2.53	1.54	1.49
5	R	550	INO	O4-N1	-2.47	1.32	1.37
5	P	550	INO	O2-C7	-2.39	1.23	1.30
5	Q	550	INO	C4-C7	2.38	1.54	1.49
5	O	550	INO	C4-C7	2.29	1.54	1.49
5	R	550	INO	O3-C2	-2.29	1.26	1.32
5	N	550	INO	O2-C7	-2.26	1.23	1.30
5	Q	550	INO	O4-N1	-2.17	1.33	1.37
5	O	550	INO	O2-C7	-2.16	1.24	1.30
5	R	550	INO	C4-C7	2.15	1.54	1.49
5	O	550	INO	C5-C4	2.08	1.42	1.39
5	P	550	INO	C3-C4	2.06	1.42	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	550	INO	O2-C7	-2.03	1.24	1.30
5	N	550	INO	C3-C4	2.03	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	INO	O2-C7-O1	-3.11	116.67	123.35
5	Q	550	INO	O2-C7-O1	-3.06	116.77	123.35
5	N	550	INO	O2-C7-C4	2.80	122.01	114.84
5	O	550	INO	O2-C7-O1	-2.79	117.36	123.35
5	R	550	INO	O2-C7-O1	-2.72	117.50	123.35
5	O	550	INO	O2-C7-C4	2.62	121.56	114.84
5	Q	550	INO	O2-C7-C4	2.56	121.40	114.84
5	P	550	INO	O2-C7-C4	2.44	121.11	114.84
5	P	550	INO	O2-C7-O1	-2.40	118.19	123.35
5	R	550	INO	O2-C7-C4	2.39	120.96	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550	INO	1	0
3	P	575	CYN	1	0
3	R	575	CYN	2	0
3	Q	575	CYN	2	0
3	O	575	CYN	1	0
5	Q	550	INO	2	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.