



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:08 am GMT

PDB ID : 3PCL  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

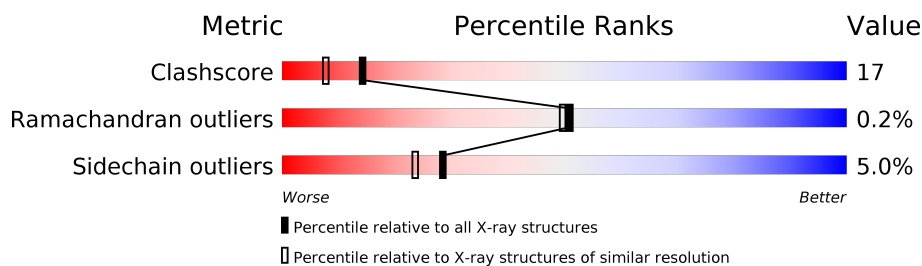
# 1 Overall quality at a glance

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	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	69% 26% 5%
1	B	200	69% 26% . .
1	C	200	65% 32% .
1	D	200	69% 27% 5% .
1	E	200	62% 32% 5% .
1	F	200	58% 36% 6% .
2	M	238	66% 28% . .

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Mol	Chain	Length	Quality of chain
2	N	238	 66% 26% 5% .
2	O	238	 64% 28% . . .
2	P	238	 61% 34% . . .
2	Q	238	 61% 31% 5% . .
2	R	238	 63% 28% 5% . .

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.

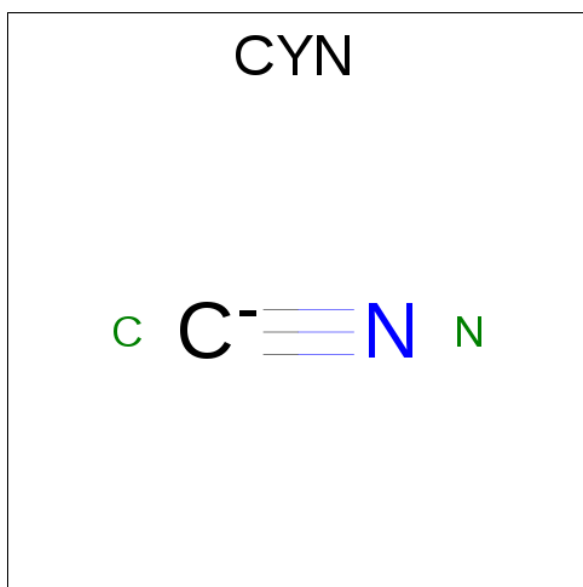
- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 (three-letter code: CYN) (formula: CN).

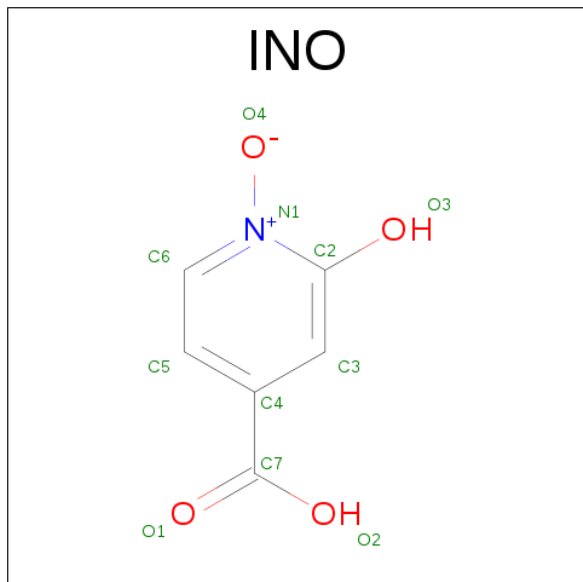


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	N	0	0
			2	1	1		
3	N	1	Total	C	N	0	0
			2	1	1		
3	O	1	Total	C	N	0	0
			2	1	1		
3	P	1	Total	C	N	0	0
			2	1	1		
3	Q	1	Total	C	N	0	0
			2	1	1		
3	R	1	Total	C	N	0	0
			2	1	1		

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

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

- Molecule 5 is 2-HYDROXYISONICOTINIC ACID N-OXIDE (three-letter code: 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	B	78	Total	O	0	0
			78	78		
6	C	79	Total	O	0	0
			79	79		
6	D	78	Total	O	0	0
			78	78		

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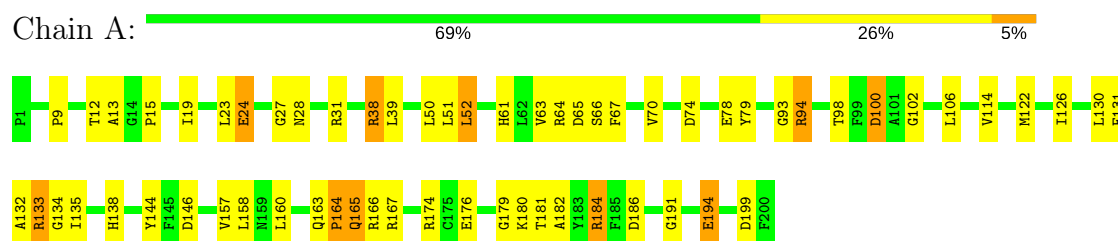
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	76	Total 76	O 76	0	0
6	F	82	Total 82	O 82	0	0
6	M	156	Total 156	O 156	0	0
6	N	159	Total 159	O 159	0	0
6	O	157	Total 157	O 157	0	0
6	P	152	Total 152	O 152	0	0
6	Q	165	Total 165	O 165	0	0
6	R	152	Total 152	O 152	0	0

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

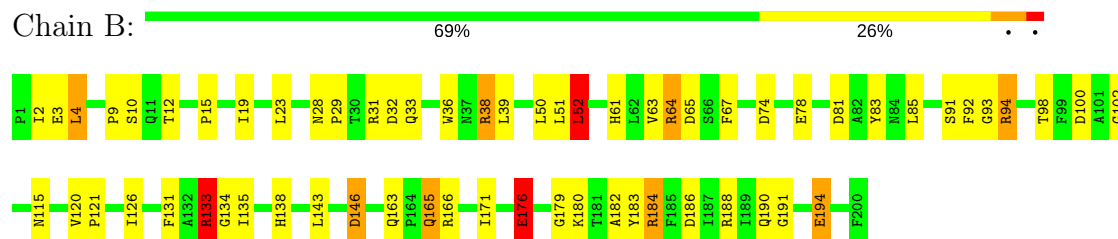
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

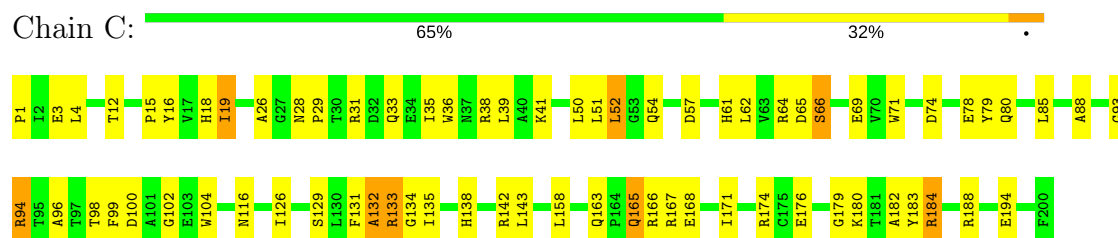
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



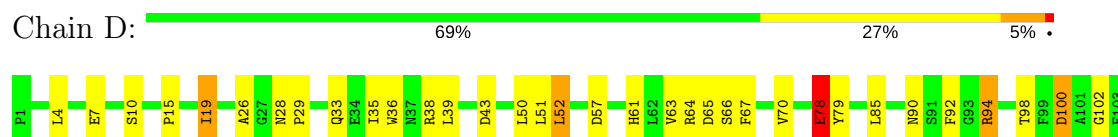
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

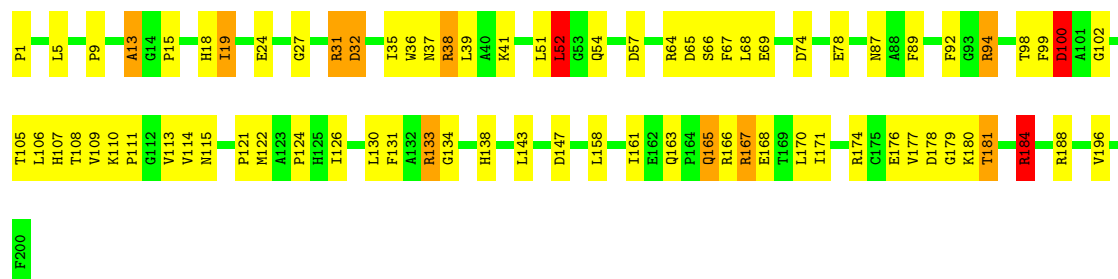






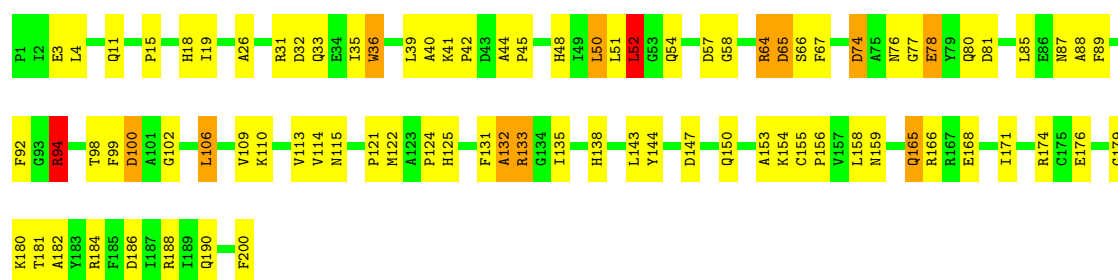
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 62% 32% 5%



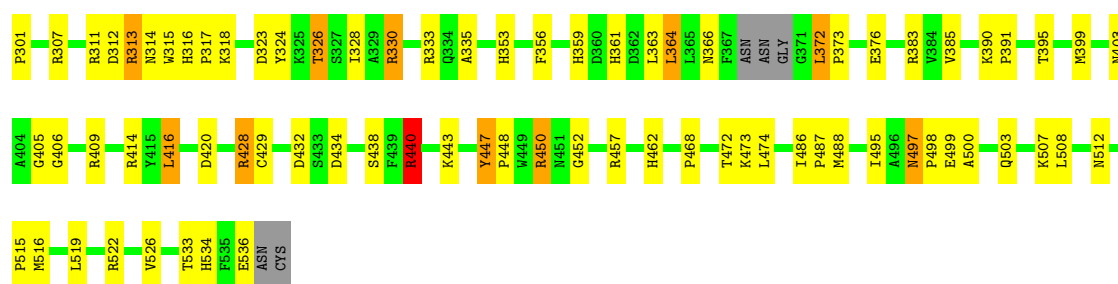
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 58% 36% 6%



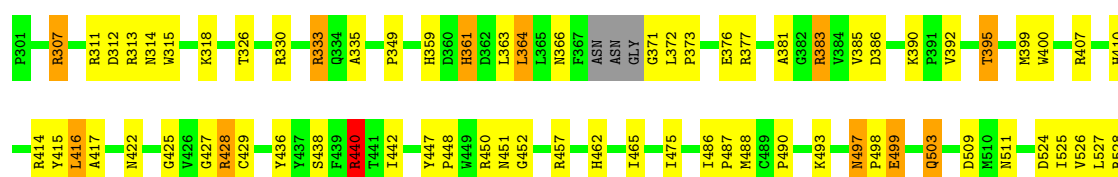
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

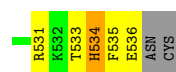
Chain M: 66% 28% 6%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

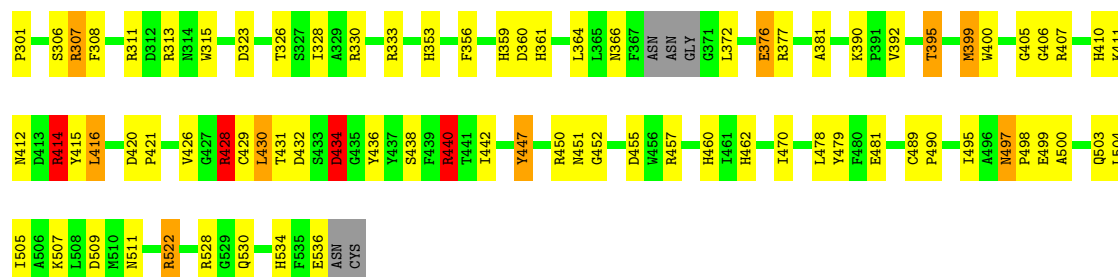
Chain N: 66% 26% 5%





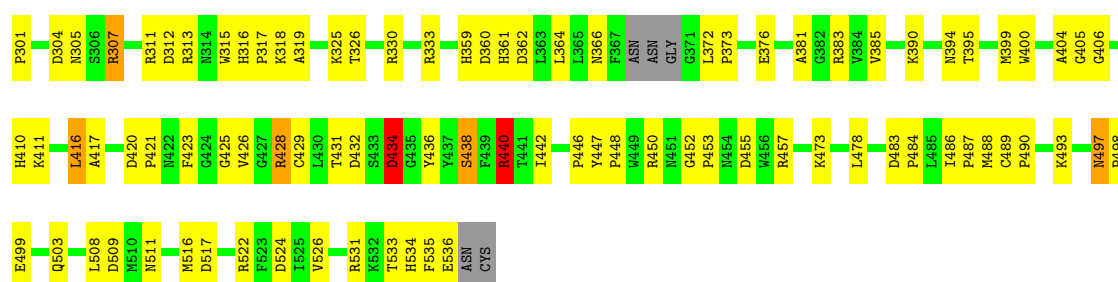
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O: 64% 28%



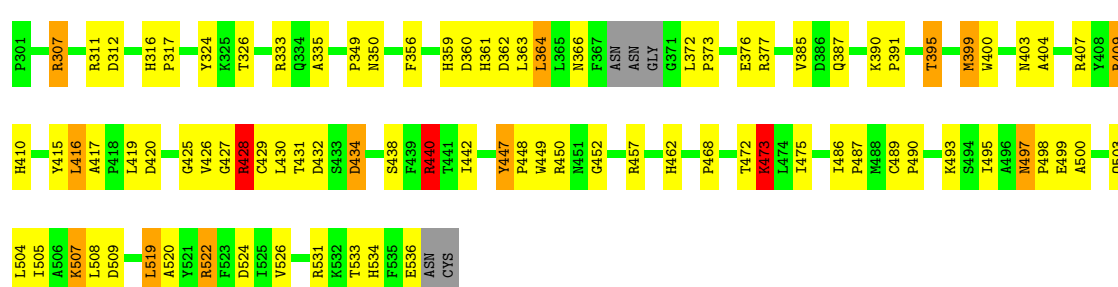
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 61% 34%



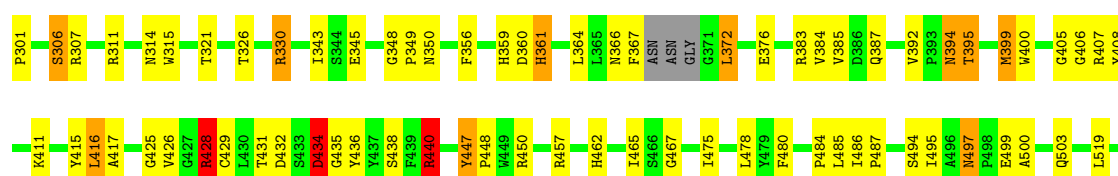
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 61% 31% 5%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 63% 28% 5%



R522	F523	D524	I525	V526	L527	Q530	R531	K532	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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: INO, CYN, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.01	2/1611 (0.1%)	1.73	25/2195 (1.1%)
1	B	1.05	2/1611 (0.1%)	1.81	33/2195 (1.5%)
1	C	1.01	1/1611 (0.1%)	1.58	22/2195 (1.0%)
1	D	1.02	1/1611 (0.1%)	1.66	24/2195 (1.1%)
1	E	1.00	0/1611	1.60	25/2195 (1.1%)
1	F	1.07	0/1611	1.66	25/2195 (1.1%)
2	M	1.10	0/1895	1.62	24/2580 (0.9%)
2	N	1.10	1/1895 (0.1%)	1.69	33/2580 (1.3%)
2	O	1.16	3/1895 (0.2%)	1.71	38/2580 (1.5%)
2	P	1.13	2/1895 (0.1%)	1.74	33/2580 (1.3%)
2	Q	1.15	1/1895 (0.1%)	1.77	33/2580 (1.3%)
2	R	1.13	1/1895 (0.1%)	1.69	27/2580 (1.0%)
All	All	1.08	14/21036 (0.1%)	1.69	342/28650 (1.2%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	313	ARG	NE-CZ	7.55	1.42	1.33
2	Q	428	ARG	CD-NE	-6.72	1.35	1.46
2	O	428	ARG	CD-NE	-6.05	1.36	1.46
1	D	10	SER	CA-CB	5.77	1.61	1.52
2	P	440	ARG	CD-NE	-5.76	1.36	1.46
1	B	94	ARG	CD-NE	-5.63	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	428	ARG	CD-NE	-5.59	1.36	1.46
1	A	94	ARG	CD-NE	-5.56	1.37	1.46
2	O	481	GLU	CD-OE2	-5.51	1.19	1.25
1	B	133	ARG	CD-NE	-5.13	1.37	1.46
1	A	133	ARG	CD-NE	-5.05	1.37	1.46
2	N	452	GLY	N-CA	5.05	1.53	1.46
1	C	194	GLU	CD-OE2	-5.03	1.20	1.25
2	R	467	GLY	N-CA	5.02	1.53	1.46

All (342) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	440	ARG	NE-CZ-NH2	-21.65	109.48	120.30
1	B	133	ARG	NE-CZ-NH1	21.22	130.91	120.30
2	N	440	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	A	94	ARG	NE-CZ-NH1	18.80	129.70	120.30
2	Q	428	ARG	CD-NE-CZ	18.64	149.70	123.60
1	D	94	ARG	NE-CZ-NH2	-18.55	111.03	120.30
1	F	94	ARG	NE-CZ-NH1	18.13	129.36	120.30
1	A	94	ARG	CD-NE-CZ	17.30	147.82	123.60
1	B	133	ARG	NE-CZ-NH2	-17.16	111.72	120.30
2	Q	440	ARG	NE-CZ-NH2	-17.00	111.80	120.30
1	D	94	ARG	NE-CZ-NH1	16.44	128.52	120.30
1	B	133	ARG	CD-NE-CZ	16.33	146.46	123.60
2	M	440	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	B	94	ARG	NE-CZ-NH1	15.56	128.08	120.30
2	O	428	ARG	CD-NE-CZ	15.50	145.31	123.60
1	B	94	ARG	CD-NE-CZ	15.32	145.05	123.60
2	R	440	ARG	NE-CZ-NH2	-14.36	113.12	120.30
1	E	94	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	A	94	ARG	NE-CZ-NH2	-13.82	113.39	120.30
2	R	407	ARG	NE-CZ-NH1	13.67	127.14	120.30
1	B	94	ARG	NE-CZ-NH2	-13.47	113.57	120.30
1	F	64	ARG	NE-CZ-NH1	-13.44	113.58	120.30
2	O	440	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	A	133	ARG	CD-NE-CZ	13.08	141.92	123.60
2	Q	428	ARG	NE-CZ-NH1	13.08	126.84	120.30
2	P	428	ARG	NE-CZ-NH1	12.91	126.75	120.30
2	Q	428	ARG	NE-CZ-NH2	-12.65	113.98	120.30
1	A	184	ARG	NE-CZ-NH2	-12.55	114.03	120.30
2	O	330	ARG	NE-CZ-NH2	-12.54	114.03	120.30
2	Q	407	ARG	NE-CZ-NH1	12.46	126.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	A	133	ARG	NE-CZ-NH2	-11.95	114.33	120.30
2	Q	457	ARG	NE-CZ-NH1	11.92	126.26	120.30
2	P	440	ARG	NE-CZ-NH1	11.77	126.19	120.30
1	A	184	ARG	NE-CZ-NH1	11.71	126.16	120.30
2	N	428	ARG	CD-NE-CZ	11.68	139.95	123.60
2	R	428	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	F	94	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	D	133	ARG	NE-CZ-NH2	-11.55	114.52	120.30
2	R	522	ARG	NE-CZ-NH1	-11.44	114.58	120.30
1	C	184	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	R	428	ARG	NE-CZ-NH2	-11.03	114.78	120.30
2	N	428	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	133	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	184	ARG	CD-NE-CZ	10.22	137.90	123.60
1	E	133	ARG	NE-CZ-NH2	-10.20	115.20	120.30
2	O	428	ARG	NE-CZ-NH1	10.15	125.38	120.30
2	N	450	ARG	NE-CZ-NH1	10.08	125.34	120.30
2	P	313	ARG	NE-CZ-NH1	10.01	125.30	120.30
2	P	307	ARG	NE-CZ-NH2	-10.00	115.30	120.30
2	R	407	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	D	167	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	M	450	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	94	ARG	CG-CD-NE	9.70	132.17	111.80
1	B	64	ARG	NE-CZ-NH1	-9.57	115.52	120.30
1	F	94	ARG	CD-NE-CZ	9.55	136.97	123.60
1	A	166	ARG	NE-CZ-NH2	-9.31	115.64	120.30
2	N	457	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	D	186	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	31	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	D	184	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	D	94	ARG	CD-NE-CZ	9.07	136.30	123.60
2	Q	440	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	O	450	ARG	NE-CZ-NH1	8.99	124.80	120.30
2	O	428	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	Q	524	ASP	CB-CG-OD2	-8.93	110.27	118.30
2	P	428	ARG	CG-CD-NE	8.91	130.51	111.80
2	P	428	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	Q	531	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	E	94	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	94	ARG	CG-CD-NE	8.70	130.07	111.80
2	N	311	ARG	NE-CZ-NH1	8.68	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	524	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	D	184	ARG	NE-CZ-NH1	8.55	124.57	120.30
2	O	407	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	M	432	ASP	CB-CG-OD1	8.48	125.93	118.30
2	N	311	ARG	NE-CZ-NH2	-8.39	116.11	120.30
2	N	440	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	P	428	ARG	CD-NE-CZ	8.24	135.13	123.60
2	Q	333	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	P	509	ASP	CB-CG-OD1	8.22	125.70	118.30
2	Q	311	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	74	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	M	330	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	R	457	ARG	CD-NE-CZ	8.17	135.03	123.60
2	Q	377	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	166	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	Q	457	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	F	133	ARG	CD-NE-CZ	-8.11	112.25	123.60
2	P	457	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	Q	407	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	O	313	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	E	31	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	D	38	ARG	NE-CZ-NH2	-7.96	116.32	120.30
2	N	307	ARG	NE-CZ-NH2	-7.95	116.32	120.30
2	R	440	ARG	NE-CZ-NH1	7.95	124.27	120.30
1	E	64	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	C	166	ARG	NE-CZ-NH2	-7.93	116.34	120.30
2	N	450	ARG	NE-CZ-NH2	-7.75	116.42	120.30
2	P	307	ARG	NE-CZ-NH1	7.72	124.16	120.30
2	P	434	ASP	CB-CG-OD2	-7.72	111.36	118.30
2	O	509	ASP	CB-CG-OD1	7.70	125.23	118.30
2	N	528	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	O	428	ARG	CG-CD-NE	7.65	127.86	111.80
1	B	74	ASP	CB-CG-OD1	7.64	125.18	118.30
2	P	440	ARG	CD-NE-CZ	7.64	134.30	123.60
2	P	432	ASP	CB-CG-OD1	7.59	125.13	118.30
1	C	94	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	N	457	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	O	377	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	F	64	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	M	450	ARG	NE-CZ-NH2	-7.53	116.53	120.30
2	O	407	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	94	ARG	CB-CG-CD	7.41	130.86	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	311	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	F	66	SER	N-CA-CB	7.34	121.51	110.50
1	F	133	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	O	528	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	F	36	TRP	CB-CA-C	7.27	124.95	110.40
1	C	94	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	B	176	GLU	OE1-CD-OE2	-7.25	114.60	123.30
1	F	64	ARG	CD-NE-CZ	-7.24	113.46	123.60
1	D	186	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	E	188	ARG	NE-CZ-NH1	7.19	123.89	120.30
2	P	483	ASP	CB-CG-OD2	7.18	124.77	118.30
1	C	133	ARG	NE-CZ-NH1	7.17	123.89	120.30
2	Q	432	ASP	CB-CG-OD2	-7.16	111.85	118.30
2	M	432	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	133	ARG	N-CA-CB	-7.13	97.77	110.60
1	B	166	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	E	174	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	74	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	174	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	N	509	ASP	CB-CG-OD1	7.07	124.67	118.30
1	B	81	ASP	CB-CG-OD1	7.05	124.65	118.30
2	P	333	ARG	CD-NE-CZ	-7.04	113.75	123.60
1	D	133	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	E	184	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	F	166	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	74	ASP	CB-CG-OD1	6.90	124.51	118.30
2	P	524	ASP	CB-CG-OD2	-6.90	112.09	118.30
2	N	333	ARG	NE-CZ-NH2	-6.90	116.85	120.30
2	Q	312	ASP	CB-CG-OD1	6.88	124.49	118.30
2	O	333	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	N	312	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	R	457	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	R	531	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	N	383	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	Q	522	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	31	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	R	450	ARG	CD-NE-CZ	-6.77	114.12	123.60
2	R	311	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	133	ARG	CD-NE-CZ	6.74	133.03	123.60
2	M	326	THR	CA-CB-CG2	-6.73	102.98	112.40
2	Q	409	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	M	428	ARG	CD-NE-CZ	6.72	133.01	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	312	ASP	CB-CG-OD1	6.70	124.33	118.30
2	M	457	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	78	GLU	OE1-CD-OE2	6.69	131.33	123.30
2	O	307	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	142	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	R	434	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	B	64	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	C	184	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	P	333	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	P	311	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	F	57	ASP	CB-CG-OD1	6.56	124.21	118.30
2	R	522	ARG	CD-NE-CZ	-6.54	114.44	123.60
2	O	432	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	D	174	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	Q	438	SER	N-CA-CB	6.50	120.25	110.50
1	C	31	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	M	440	ARG	NH1-CZ-NH2	6.47	126.52	119.40
1	C	167	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	N	531	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	O	450	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	P	428	ARG	CB-CG-CD	6.44	128.35	111.60
2	R	330	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	158	LEU	CB-CA-C	6.42	122.39	110.20
2	N	407	ARG	CD-NE-CZ	-6.41	114.62	123.60
2	M	312	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	O	353	HIS	CA-CB-CG	-6.39	102.73	113.60
2	M	372	LEU	CA-CB-CG	6.39	130.00	115.30
2	M	450	ARG	CD-NE-CZ	6.39	132.54	123.60
2	Q	434	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	O	434	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	F	186	ASP	CB-CG-OD1	6.36	124.03	118.30
2	Q	417	ALA	CB-CA-C	6.36	119.64	110.10
2	N	503	GLN	CA-CB-CG	6.36	127.38	113.40
1	E	133	ARG	CA-CB-CG	6.35	127.36	113.40
2	P	517	ASP	CB-CG-OD1	6.30	123.97	118.30
2	P	531	ARG	CA-CB-CG	6.29	127.24	113.40
1	A	146	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	176	GLU	CG-CD-OE1	6.24	130.78	118.30
2	P	372	LEU	CB-CA-C	6.23	122.04	110.20
1	B	83	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	F	74	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	E	100	ASP	CB-CG-OD2	6.19	123.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	524	ASP	CB-CG-OD1	6.18	123.86	118.30
2	P	517	ASP	CB-CG-OD2	-6.17	112.74	118.30
2	N	499	GLU	CG-CD-OE1	6.17	130.63	118.30
1	E	32	ASP	CB-CG-OD2	-6.15	112.76	118.30
2	R	432	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	E	38	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	F	57	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	94	ARG	CB-CG-CD	6.14	127.56	111.60
1	C	133	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	188	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	57	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	96	ALA	N-CA-CB	-6.06	101.61	110.10
1	D	36	TRP	CB-CA-C	6.06	122.52	110.40
1	B	188	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	38	ARG	CD-NE-CZ	-6.00	115.19	123.60
1	B	176	GLU	CB-CG-CD	6.00	130.39	114.20
2	P	383	ARG	CD-NE-CZ	-6.00	115.20	123.60
2	Q	434	ASP	CA-CB-CG	-6.00	100.21	113.40
2	N	524	ASP	CB-CG-OD2	-5.97	112.92	118.30
2	R	438	SER	N-CA-CB	5.97	119.46	110.50
1	B	133	ARG	CA-CB-CG	5.96	126.51	113.40
2	O	307	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	Q	420	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	94	ARG	CG-CD-NE	5.94	124.27	111.80
1	C	62	LEU	CA-CB-CG	5.93	128.95	115.30
2	P	450	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	N	531	ARG	CD-NE-CZ	5.93	131.90	123.60
2	O	522	ARG	NE-CZ-NH1	-5.93	117.34	120.30
2	P	457	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	R	524	ASP	CB-CG-OD1	5.89	123.60	118.30
2	O	311	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	52	LEU	CA-CB-CG	5.87	128.80	115.30
2	M	333	ARG	CD-NE-CZ	-5.84	115.42	123.60
1	A	186	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	M	447	TYR	N-CA-CB	-5.80	100.16	110.60
2	O	447	TYR	N-CA-CB	-5.80	100.16	110.60
2	P	312	ASP	CB-CG-OD1	5.80	123.52	118.30
1	E	94	ARG	CD-NE-CZ	5.79	131.71	123.60
2	Q	428	ARG	CG-CD-NE	5.79	123.96	111.80
1	E	167	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	94	ARG	CG-CD-NE	5.78	123.93	111.80
2	P	432	ASP	CB-CG-OD2	-5.77	113.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	414	ARG	CD-NE-CZ	-5.76	115.53	123.60
2	Q	307	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	N	534	HIS	N-CA-CB	5.75	120.95	110.60
1	E	38	ARG	CD-NE-CZ	-5.75	115.56	123.60
1	C	167	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	23	LEU	CB-CA-C	5.72	121.07	110.20
2	O	457	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	E	184	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	E	166	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	186	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	69	GLU	N-CA-CB	5.68	120.83	110.60
2	N	524	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	183	TYR	N-CA-CB	5.67	120.81	110.60
2	M	438	SER	N-CA-CB	5.67	119.00	110.50
2	O	457	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	N	361	HIS	CA-CB-CG	-5.64	104.02	113.60
1	E	52	LEU	CB-CA-C	5.63	120.90	110.20
2	P	452	GLY	N-CA-C	-5.62	99.04	113.10
1	B	36	TRP	CB-CA-C	5.60	121.61	110.40
2	O	504	LEU	CA-CB-CG	5.60	128.17	115.30
2	M	313	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	F	133	ARG	CA-CB-CG	5.58	125.68	113.40
2	Q	508	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	E	31	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	F	188	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	O	360	ASP	CB-CG-OD2	-5.55	113.30	118.30
2	O	376	GLU	CG-CD-OE2	-5.55	107.20	118.30
2	N	452	GLY	N-CA-C	-5.53	99.27	113.10
1	A	174	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	129	SER	N-CA-CB	5.52	118.79	110.50
1	E	13	ALA	CB-CA-C	5.50	118.35	110.10
2	P	455	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	D	57	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	D	133	ARG	N-CA-CB	-5.45	100.79	110.60
2	N	312	ASP	CB-CG-OD1	5.44	123.20	118.30
1	F	158	LEU	CB-CA-C	5.44	120.53	110.20
1	A	194	GLU	CG-CD-OE2	5.43	129.15	118.30
1	E	57	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	78	GLU	OE1-CD-OE2	5.42	129.81	123.30
2	M	383	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	R	432	ASP	CB-CG-OD1	5.42	123.17	118.30
2	M	414	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	447	TYR	N-CA-CB	-5.40	100.88	110.60
1	D	106	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	146	ASP	CB-CG-OD1	5.36	123.13	118.30
2	M	452	GLY	N-CA-C	-5.36	99.70	113.10
1	B	194	GLU	OE1-CD-OE2	5.34	129.70	123.30
2	Q	324	TYR	CB-CG-CD1	-5.33	117.80	121.00
2	R	376	GLU	CG-CD-OE2	-5.33	107.64	118.30
1	B	184	ARG	CG-CD-NE	-5.32	100.62	111.80
1	E	166	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	81	ASP	CB-CG-OD2	-5.31	113.53	118.30
1	B	10	SER	CB-CA-C	-5.30	100.02	110.10
1	A	167	ARG	CD-NE-CZ	-5.29	116.19	123.60
1	F	78	GLU	CG-CD-OE1	5.29	128.88	118.30
1	E	64	ARG	CD-NE-CZ	-5.29	116.20	123.60
2	P	450	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	13	ALA	N-CA-CB	5.29	117.50	110.10
1	C	133	ARG	N-CA-CB	-5.29	101.08	110.60
2	O	522	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	Q	519	LEU	CB-CG-CD2	-5.26	102.05	111.00
2	Q	452	GLY	N-CA-C	-5.26	99.94	113.10
1	C	174	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	R	480	PHE	CB-CG-CD1	-5.26	117.12	120.80
2	N	314	ASN	CB-CA-C	5.25	120.90	110.40
2	Q	447	TYR	N-CA-CB	-5.25	101.15	110.60
1	C	57	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	167	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	O	323	ASP	CB-CG-OD1	5.24	123.02	118.30
1	F	11	GLN	O-C-N	5.22	131.06	122.70
2	O	434	ASP	CA-CB-CG	-5.21	101.94	113.40
2	N	428	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	O	430	LEU	N-CA-CB	-5.19	100.01	110.40
2	O	447	TYR	CB-CG-CD2	5.19	124.12	121.00
1	F	52	LEU	CA-CB-CG	5.19	127.23	115.30
2	R	361	HIS	CA-CB-CG	-5.18	104.79	113.60
2	Q	311	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	7	GLU	OE1-CD-OE2	5.17	129.51	123.30
1	F	78	GLU	N-CA-CB	5.16	119.89	110.60
1	B	183	TYR	N-CA-CB	5.16	119.88	110.60
2	Q	387	GLN	O-C-N	5.14	130.93	122.70
1	F	65	ASP	CB-CG-OD1	5.13	122.92	118.30
2	R	314	ASN	N-CA-CB	5.12	119.83	110.60
1	A	38	ARG	CD-NE-CZ	-5.12	116.44	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	353	HIS	CA-CB-CG	-5.11	104.91	113.60
2	N	377	ARG	CD-NE-CZ	5.11	130.75	123.60
1	C	188	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	N	451	ASN	CB-CA-C	5.08	120.56	110.40
2	M	311	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	M	323	ASP	CB-CG-OD1	5.08	122.87	118.30
2	O	377	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	N	414	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	Q	473	LYS	CA-CB-CG	5.07	124.56	113.40
2	O	452	GLY	N-CA-C	-5.07	100.43	113.10
2	O	430	LEU	CB-CA-C	5.07	119.83	110.20
2	N	509	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	D	57	ASP	CB-CA-C	5.04	120.49	110.40
2	O	447	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	F	106	LEU	N-CA-CB	-5.03	100.35	110.40
1	B	52	LEU	CB-CA-C	5.02	119.73	110.20
2	R	367	PHE	CA-C-O	-5.01	109.58	120.10
1	F	188	ARG	CB-CA-C	5.00	120.40	110.40

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	48	0
1	B	1571	0	1499	52	0
1	C	1571	0	1499	57	0
1	D	1571	0	1499	55	0
1	E	1571	0	1499	70	0
1	F	1571	0	1499	86	0
2	M	1840	0	1794	67	0
2	N	1840	0	1794	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1840	0	1794	62	0
2	P	1840	0	1794	77	0
2	Q	1840	0	1794	75	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
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	6	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	702	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 17.

All (702) 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	1.10
1:B:165:GLN:NE2	1:B:165:GLN:H	1.52	1.06
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.44	0.99
1:E:165:GLN:H	1:E:165:GLN:HE21	1.02	0.97
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.45	0.95
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.47	0.95
2:R:497:ASN:HD22	2:R:499:GLU:H	1.08	0.93
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.49	0.93
2:R:361:HIS:H	2:R:361:HIS:CD2	1.84	0.93
1:E:165:GLN:NE2	1:E:165:GLN:H	1.66	0.92
2:P:390:LYS:HD2	6:P:647:HOH:O	1.68	0.92
1:B:165:GLN:HE21	1:B:165:GLN:H	0.92	0.91
1:B:165:GLN:N	1:B:165:GLN:HE21	1.68	0.91
2:R:497:ASN:ND2	2:R:499:GLU:H	1.67	0.90
2:M:390:LYS:HD2	6:M:641:HOH:O	1.72	0.90
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.55	0.88
1:F:176:GLU:HG3	1:F:180:LYS:O	1.73	0.88
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.56	0.88
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.56	0.87
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.56	0.86
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
1:F:165:GLN:HE21	1:F:165:GLN:H	1.24	0.86
1:C:64:ARG:NH2	1:C:100:ASP:O	2.09	0.85
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.59	0.85
1:D:64:ARG:NH2	1:D:100:ASP:O	2.10	0.85
2:M:361:HIS:H	2:M:361:HIS:CD2	1.92	0.85
2:Q:356:PHE:CZ	2:Q:430:LEU:HD13	2.13	0.84
2:O:356:PHE:CD1	2:O:428:ARG:HD2	2.14	0.83
2:O:390:LYS:HD3	6:O:649:HOH:O	1.78	0.83
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.25	0.83
1:B:176:GLU:HG3	1:B:180:LYS:O	1.79	0.82
2:R:497:ASN:HD22	2:R:499:GLU:N	1.77	0.82
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.60	0.81
2:P:497:ASN:HD22	2:P:499:GLU:H	1.26	0.80
2:M:361:HIS:HD2	2:M:361:HIS:H	1.27	0.80
2:N:390:LYS:HD3	6:N:648:HOH:O	1.80	0.80
1:B:134:GLY:CA	2:N:326:THR:HG22	2.11	0.79
1:F:19:ILE:O	2:R:426:VAL:HG21	1.83	0.79
1:C:165:GLN:H	1:C:165:GLN:NE2	1.81	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:ASN:ND2	2:M:499:GLU:H	1.83	0.77
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.15	0.77
1:F:165:GLN:NE2	1:F:165:GLN:H	1.82	0.76
2:M:497:ASN:HD22	2:M:499:GLU:H	1.33	0.76
1:E:19:ILE:O	2:Q:426:VAL:HG21	1.84	0.76
2:N:307:ARG:HD2	6:N:659:HOH:O	1.84	0.76
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.66	0.76
2:R:306:SER:CB	2:R:530:GLN:HE21	1.98	0.76
2:P:416:LEU:HD23	2:P:416:LEU:C	2.07	0.75
1:B:176:GLU:OE2	1:B:179:GLY:O	2.05	0.74
2:P:497:ASN:ND2	2:P:499:GLU:H	1.86	0.74
1:C:79:TYR:O	2:O:301:PRO:HB3	1.88	0.74
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.17	0.74
1:A:78:GLU:OE1	6:A:235:HOH:O	2.06	0.73
2:N:497:ASN:HD22	2:N:499:GLU:H	1.35	0.73
2:R:536:GLU:HB2	6:R:1331:HOH:O	1.88	0.73
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.24	0.73
2:O:361:HIS:CD2	2:O:361:HIS:H	2.04	0.73
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.73
2:R:416:LEU:HD23	2:R:417:ALA:N	2.03	0.72
1:E:165:GLN:N	1:E:165:GLN:HE21	1.83	0.72
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.38	0.72
1:D:165:GLN:H	1:D:165:GLN:HE21	1.36	0.72
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.07	0.72
2:R:416:LEU:HD23	2:R:416:LEU:C	2.10	0.72
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.71	0.72
1:C:3:GLU:HA	1:C:3:GLU:OE1	1.90	0.72
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.91	0.71
1:D:165:GLN:H	1:D:165:GLN:NE2	1.89	0.71
1:C:176:GLU:HG3	1:C:180:LYS:O	1.90	0.71
2:N:416:LEU:HD23	2:N:417:ALA:N	2.06	0.71
2:M:416:LEU:C	2:M:416:LEU:HD23	2.11	0.71
2:O:497:ASN:HD22	2:O:499:GLU:H	1.36	0.71
2:O:497:ASN:ND2	2:O:499:GLU:H	1.89	0.70
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.72	0.70
1:C:165:GLN:H	1:C:165:GLN:HE21	1.36	0.70
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.73	0.70
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.19	0.70
2:P:416:LEU:HD23	2:P:417:ALA:N	2.05	0.70
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.39	0.70
2:R:356:PHE:CD2	2:R:428:ARG:HD3	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.92	0.69
1:D:78:GLU:CG	2:P:301:PRO:HG2	2.22	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:HH12	1.58	0.69
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.07	0.69
1:F:113:VAL:HG13	1:F:122:MET:O	1.93	0.68
1:F:51:LEU:HD12	1:F:106:LEU:HD23	1.74	0.68
2:O:390:LYS:HE2	6:O:728:HOH:O	1.92	0.68
2:P:497:ASN:HD22	2:P:499:GLU:N	1.91	0.68
2:Q:356:PHE:HD1	2:Q:428:ARG:HD2	1.59	0.68
1:D:176:GLU:HG3	1:D:180:LYS:O	1.93	0.68
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.76	0.68
2:N:361:HIS:H	2:N:361:HIS:CD2	2.10	0.67
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.27	0.67
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.75	0.67
2:N:488:MET:CE	1:C:1:PRO:HG3	2.24	0.67
2:P:361:HIS:CD2	2:P:361:HIS:H	2.11	0.67
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.27	0.66
1:F:44:ALA:O	1:F:48:HIS:NE2	2.22	0.66
1:A:165:GLN:H	1:A:165:GLN:NE2	1.94	0.66
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.11	0.66
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.10	0.65
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.60	0.65
1:B:98:THR:O	1:B:102:GLY:HA2	1.97	0.65
1:C:134:GLY:HA3	2:O:326:THR:HG22	1.79	0.65
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.79	0.65
2:R:306:SER:OG	2:R:530:GLN:NE2	2.28	0.65
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.78	0.64
2:O:356:PHE:HE1	2:O:428:ARG:HD3	1.60	0.64
1:B:64:ARG:NH2	1:B:100:ASP:O	2.29	0.64
2:M:536:GLU:HB2	6:M:697:HOH:O	1.97	0.64
2:Q:399:MET:HA	2:Q:462:HIS:O	1.98	0.64
2:Q:390:LYS:HD3	6:Q:1016:HOH:O	1.96	0.64
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.63	0.64
1:C:19:ILE:O	2:O:426:VAL:HG21	1.98	0.64
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.46	0.64
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.13	0.64
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.80	0.64
2:N:497:ASN:ND2	2:N:499:GLU:H	1.96	0.64
2:N:416:LEU:C	2:N:416:LEU:HD23	2.19	0.63
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASP:OD2	1:C:133:ARG:HD3	1.99	0.63
2:N:364:LEU:CD2	2:N:440:ARG:HD3	2.27	0.63
1:E:69:GLU:OE1	2:Q:473:LYS:HE2	1.98	0.63
2:R:400:TRP:HA	2:R:425:GLY:O	1.99	0.63
2:R:406:GLY:O	2:R:447:TYR:HD1	1.82	0.63
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.14	0.63
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.81	0.63
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.28	0.62
2:M:359:HIS:O	2:M:366:ASN:HB3	1.99	0.62
2:M:497:ASN:HD22	2:M:497:ASN:C	2.01	0.62
1:D:33:GLN:HB3	1:D:85:LEU:HD11	1.82	0.62
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.81	0.62
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.15	0.62
2:R:531:ARG:NH1	2:R:532:LYS:O	2.33	0.62
2:Q:356:PHE:CD1	2:Q:428:ARG:HD2	2.35	0.62
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.35	0.62
1:F:50:LEU:HD23	1:F:182:ALA:HB2	1.82	0.61
2:Q:390:LYS:HE2	6:Q:1133:HOH:O	1.98	0.61
2:O:361:HIS:HD2	2:O:361:HIS:H	1.48	0.61
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.25	0.61
1:E:134:GLY:HA3	2:Q:326:THR:CG2	2.24	0.61
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.14	0.61
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.98	0.61
1:F:19:ILE:HD11	2:R:408:TYR:HD1	1.65	0.61
2:O:359:HIS:O	2:O:366:ASN:HB3	2.01	0.61
2:R:399:MET:HA	2:R:462:HIS:O	2.01	0.61
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.36	0.61
2:N:385:VAL:O	2:N:526:VAL:HA	2.01	0.61
1:E:134:GLY:CA	2:Q:326:THR:HG22	2.25	0.61
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.36	0.60
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.49	0.60
2:M:326:THR:CG2	2:M:330:ARG:HD2	2.32	0.60
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.22	0.60
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.37	0.60
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.02	0.60
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.02	0.60
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.48	0.60
1:A:134:GLY:HA3	2:M:326:THR:CG2	2.32	0.59
1:D:98:THR:O	1:D:102:GLY:HA2	2.03	0.59
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.02	0.59
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.37	0.59
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.18	0.59
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.01	0.59
1:B:134:GLY:HA3	2:N:326:THR:CG2	2.22	0.59
2:R:364:LEU:HD22	2:R:440:ARG:CD	2.29	0.59
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.37	0.59
2:P:361:HIS:HD2	2:P:361:HIS:H	1.48	0.59
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.67	0.59
1:E:98:THR:O	1:E:102:GLY:HA2	2.02	0.59
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.03	0.59
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.33	0.59
2:N:390:LYS:HE2	6:N:726:HOH:O	2.03	0.59
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.85	0.58
2:O:497:ASN:HD22	2:O:497:ASN:C	2.07	0.58
1:C:64:ARG:NE	1:C:100:ASP:O	2.36	0.58
2:R:385:VAL:O	2:R:526:VAL:HA	2.02	0.58
2:R:392:VAL:HG12	2:R:395:THR:HB	1.83	0.58
1:B:28:ASN:HB3	1:B:29:PRO:HD2	1.84	0.58
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.65	0.58
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.49	0.58
2:P:362:ASP:OD1	2:P:440:ARG:HD2	2.04	0.58
2:R:361:HIS:N	2:R:361:HIS:CD2	2.57	0.58
1:E:113:VAL:HG23	1:E:124:PRO:HG3	1.84	0.58
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.39	0.58
2:N:313:ARG:O	2:N:318:LYS:HE2	2.04	0.58
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.04	0.58
1:F:58:GLY:HA3	1:F:190:GLN:OE1	2.03	0.58
2:Q:473:LYS:NZ	6:Q:1032:HOH:O	2.36	0.58
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.04	0.58
2:M:376:GLU:HG2	2:P:446:PRO:HD2	1.86	0.57
2:P:376:GLU:O	2:P:442:ILE:HA	2.04	0.57
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.34	0.57
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.32	0.57
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.87	0.57
1:E:15:PRO:HD2	3:Q:575:CYN:N	2.19	0.57
1:E:176:GLU:HA	1:E:180:LYS:O	2.04	0.57
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.20	0.57
1:D:52:LEU:HA	1:D:104:TRP:O	2.04	0.57
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.87	0.57
2:Q:307:ARG:HD2	6:Q:1037:HOH:O	2.05	0.57
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:GLU:HG3	1:B:180:LYS:C	2.24	0.56
1:D:100:ASP:N	1:D:100:ASP:OD1	2.37	0.56
2:O:356:PHE:CE1	2:O:428:ARG:CD	2.87	0.56
1:F:155:CYS:O	1:F:159:ASN:ND2	2.38	0.56
1:E:161:ILE:O	1:E:167:ARG:NH2	2.34	0.56
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.87	0.56
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.41	0.56
1:A:100:ASP:OD1	1:A:100:ASP:N	2.38	0.56
2:Q:409:ARG:HA	2:Q:419:LEU:HD21	1.87	0.56
2:N:381:ALA:HB2	2:N:438:SER:HB2	1.87	0.56
2:Q:497:ASN:HD21	2:Q:499:GLU:HB2	1.68	0.56
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.70	0.56
1:D:33:GLN:HB3	1:D:85:LEU:CD1	2.36	0.56
2:Q:522:ARG:NH1	6:Q:1053:HOH:O	2.38	0.56
1:F:110:LYS:NZ	1:F:147:ASP:OD1	2.35	0.56
1:D:131:PHE:CE1	1:D:138:HIS:HB3	2.41	0.56
2:M:473:LYS:HD2	2:M:474:LEU:N	2.21	0.55
2:R:497:ASN:ND2	2:R:499:GLU:N	2.44	0.55
1:B:165:GLN:N	1:B:165:GLN:NE2	2.36	0.55
2:R:394:ASN:HA	2:R:431:THR:O	2.07	0.55
1:F:131:PHE:O	1:F:132:ALA:HB2	2.07	0.55
2:R:356:PHE:CE2	2:R:428:ARG:HD3	2.41	0.55
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.88	0.55
1:A:176:GLU:HA	1:A:180:LYS:O	2.06	0.55
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.69	0.55
1:D:134:GLY:HA3	2:P:326:THR:CG2	2.34	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	0.54
2:M:448:PRO:HB2	2:P:516:MET:HA	1.88	0.54
2:Q:356:PHE:HZ	2:Q:430:LEU:HD13	1.70	0.54
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.54
1:D:51:LEU:O	1:D:105:THR:HA	2.08	0.54
1:A:176:GLU:HG2	1:A:179:GLY:HA2	1.87	0.54
1:C:64:ARG:CZ	1:C:100:ASP:O	2.55	0.54
1:E:68:LEU:N	1:E:68:LEU:HD12	2.22	0.54
2:O:505:ILE:HG22	2:O:507:LYS:CE	2.38	0.54
2:R:395:THR:HG22	2:R:431:THR:CG2	2.37	0.54
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.42	0.54
1:E:1:PRO:HB2	6:E:201:HOH:O	2.07	0.54
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.08	0.54
1:F:33:GLN:CG	1:F:85:LEU:HD12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:399:MET:HA	2:M:462:HIS:O	2.07	0.54
1:F:92:PHE:CG	2:R:349:PRO:HG3	2.43	0.54
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.43	0.54
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.43	0.54
2:M:416:LEU:CD2	2:M:416:LEU:C	2.76	0.54
1:C:100:ASP:OD1	1:C:100:ASP:N	2.40	0.53
2:M:326:THR:O	2:M:326:THR:HG22	2.07	0.53
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.90	0.53
2:M:314:ASN:OD1	2:M:318:LYS:HE2	2.07	0.53
2:P:362:ASP:OD1	2:P:364:LEU:HB2	2.08	0.53
2:Q:356:PHE:CE2	2:Q:430:LEU:HD13	2.43	0.53
1:C:16:TYR:O	1:C:19:ILE:HG23	2.08	0.53
1:E:176:GLU:HG3	1:E:180:LYS:O	2.09	0.53
2:N:361:HIS:HD2	2:N:361:HIS:H	1.55	0.53
2:O:522:ARG:NH1	6:O:672:HOH:O	2.35	0.53
1:A:28:ASN:HB3	6:A:265:HOH:O	2.08	0.53
1:D:66:SER:HA	1:D:132:ALA:HB2	1.89	0.53
1:A:79:TYR:O	2:M:301:PRO:HB2	2.08	0.53
2:Q:364:LEU:CD2	2:Q:440:ARG:HD3	2.38	0.53
1:D:191:GLY:O	1:D:194:GLU:HB2	2.09	0.53
1:D:78:GLU:CD	2:P:301:PRO:HG2	2.28	0.53
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.24	0.53
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.38	0.53
1:E:41:LYS:HD2	1:E:87:ASN:O	2.09	0.53
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.73	0.53
1:A:78:GLU:CG	2:M:301:PRO:HG3	2.39	0.53
2:O:416:LEU:C	2:O:416:LEU:HD23	2.29	0.53
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.91	0.53
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.91	0.53
1:E:52:LEU:HD23	1:E:184:ARG:NH1	2.24	0.53
2:N:359:HIS:O	2:N:366:ASN:HB3	2.08	0.53
2:R:405:GLY:HA3	6:R:1255:HOH:O	2.08	0.53
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.44	0.52
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.44	0.52
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.52
1:F:19:ILE:O	2:R:426:VAL:CG2	2.56	0.52
1:E:24:GLU:O	1:E:27:GLY:N	2.41	0.52
1:B:4:LEU:HD22	2:P:511:ASN:OD1	2.08	0.52
1:C:3:GLU:OE1	1:C:3:GLU:CA	2.51	0.52
2:M:356:PHE:HE1	2:M:428:ARG:HD2	1.73	0.52
1:C:71:TRP:CD1	2:O:470:ILE:HD13	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.10	0.52
3:R:575:CYN:C	6:R:1181:HOH:O	2.56	0.52
1:C:50:LEU:HD12	1:C:51:LEU:N	2.25	0.52
2:P:319:ALA:HB3	6:P:684:HOH:O	2.09	0.52
1:A:66:SER:HB2	1:A:130:LEU:HD11	1.92	0.52
1:B:19:ILE:CG2	2:N:410:HIS:HB2	2.40	0.52
2:O:497:ASN:HD22	2:O:498:PRO:N	2.07	0.52
2:O:505:ILE:HG22	2:O:507:LYS:HE2	1.92	0.52
2:N:363:LEU:HD11	2:N:427:GLY:HA3	1.92	0.52
1:B:143:LEU:HD23	1:B:143:LEU:C	2.30	0.52
1:D:131:PHE:CD1	1:D:138:HIS:HB3	2.45	0.52
1:E:100:ASP:OD1	1:E:100:ASP:N	2.42	0.52
1:E:92:PHE:CD1	2:Q:349:PRO:HG3	2.45	0.52
1:E:92:PHE:CG	2:Q:349:PRO:HG3	2.44	0.52
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.10	0.52
1:C:176:GLU:HA	1:C:180:LYS:O	2.10	0.52
2:M:356:PHE:CE1	2:M:428:ARG:HD2	2.45	0.52
1:C:143:LEU:HD23	1:C:143:LEU:C	2.31	0.51
1:E:176:GLU:HG3	1:E:180:LYS:C	2.31	0.51
2:M:361:HIS:N	2:M:361:HIS:CD2	2.64	0.51
2:Q:497:ASN:ND2	2:Q:499:GLU:H	2.06	0.51
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.10	0.51
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.93	0.51
1:D:134:GLY:CA	2:P:326:THR:HG22	2.35	0.51
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.24	0.51
1:E:115:ASN:HA	1:E:121:PRO:HA	1.92	0.51
1:F:174:ARG:HE	1:F:181:THR:HG23	1.75	0.51
2:O:307:ARG:HD2	6:O:661:HOH:O	2.11	0.51
2:P:362:ASP:OD2	2:P:440:ARG:NH1	2.44	0.51
2:O:505:ILE:O	2:O:507:LYS:HE3	2.11	0.51
2:P:316:HIS:HB3	2:P:317:PRO:HD2	1.93	0.51
2:P:359:HIS:O	2:P:366:ASN:HB3	2.11	0.51
1:C:78:GLU:CD	2:O:301:PRO:HG2	2.31	0.51
2:P:434:ASP:HB3	2:P:436:TYR:HD2	1.74	0.51
1:F:52:LEU:CD2	1:F:184:ARG:HH12	2.24	0.51
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.92	0.51
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.41	0.51
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.44	0.51
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	1.92	0.51
1:E:67:PHE:C	1:E:68:LEU:HD12	2.31	0.50
1:C:15:PRO:HD2	3:O:575:CYN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:390:LYS:HD3	6:M:719:HOH:O	2.10	0.50
2:M:405:GLY:HA3	6:M:644:HOH:O	2.10	0.50
2:M:328:ILE:HD12	2:N:335:ALA:HB2	1.92	0.50
2:Q:364:LEU:HD22	2:Q:440:ARG:CG	2.42	0.50
2:M:363:LEU:HD12	2:M:363:LEU:N	2.25	0.50
2:P:405:GLY:HA3	6:P:650:HOH:O	2.11	0.50
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.93	0.50
1:F:78:GLU:HB2	1:F:80:GLN:HE21	1.76	0.50
2:N:536:GLU:HB2	6:N:702:HOH:O	2.10	0.50
2:P:536:GLU:HB2	6:P:701:HOH:O	2.11	0.50
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.75	0.50
1:E:5:LEU:HG	6:Q:1093:HOH:O	2.11	0.50
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.94	0.50
1:F:19:ILE:HD11	2:R:408:TYR:CD1	2.47	0.50
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.60	0.50
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.94	0.50
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.47	0.50
1:E:177:VAL:HG12	1:E:178:ASP:OD2	2.12	0.50
2:P:533:THR:HA	6:P:632:HOH:O	2.12	0.50
1:F:50:LEU:HD23	1:F:182:ALA:CB	2.41	0.50
1:B:133:ARG:HG2	2:N:326:THR:HG21	1.93	0.50
1:B:98:THR:HB	1:B:100:ASP:OD1	2.11	0.49
2:R:359:HIS:O	2:R:366:ASN:HB3	2.12	0.49
1:C:176:GLU:HG3	1:C:180:LYS:C	2.31	0.49
1:E:18:HIS:CE1	1:E:99:PHE:CE1	3.01	0.49
1:F:48:HIS:HA	1:F:109:VAL:HG12	1.93	0.49
2:N:392:VAL:HG12	2:N:395:THR:HB	1.95	0.49
2:R:306:SER:HB3	2:R:530:GLN:HG3	1.94	0.49
2:P:305:ASN:N	6:P:733:HOH:O	2.39	0.49
2:R:536:GLU:HG3	6:R:1224:HOH:O	2.11	0.49
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.95	0.49
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.42	0.49
2:M:406:GLY:O	2:M:447:TYR:HD1	1.95	0.49
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.12	0.49
1:F:115:ASN:HA	1:F:121:PRO:HA	1.94	0.49
1:F:131:PHE:CE2	1:F:138:HIS:HB3	2.47	0.49
1:F:176:GLU:HG3	1:F:180:LYS:C	2.32	0.49
1:F:78:GLU:HB2	1:F:80:GLN:NE2	2.27	0.49
2:M:497:ASN:HD22	2:M:498:PRO:N	2.11	0.49
2:R:383:ARG:HA	2:R:435:GLY:O	2.13	0.49
1:F:36:TRP:CE3	1:F:36:TRP:HA	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.49
2:R:478:LEU:C	2:R:478:LEU:HD23	2.33	0.49
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.94	0.49
1:F:35:ILE:CG2	1:F:94:ARG:HG3	2.36	0.49
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.94	0.49
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.42	0.49
2:R:356:PHE:HD2	2:R:428:ARG:HD3	1.75	0.49
1:E:143:LEU:HD23	1:E:143:LEU:C	2.33	0.48
1:A:114:VAL:HG23	1:A:122:MET:HE2	1.95	0.48
1:E:18:HIS:CE1	1:E:99:PHE:HE1	2.31	0.48
2:N:497:ASN:HD22	2:N:497:ASN:C	2.16	0.48
1:A:114:VAL:HG23	1:A:122:MET:CE	2.44	0.48
1:C:98:THR:O	1:C:102:GLY:HA2	2.13	0.48
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.37	0.48
1:F:39:LEU:N	1:F:39:LEU:HD12	2.29	0.48
2:R:387:GLN:HG3	2:R:527:LEU:O	2.14	0.48
1:D:176:GLU:HA	1:D:180:LYS:O	2.13	0.48
2:P:497:ASN:HD21	2:P:499:GLU:HB2	1.76	0.48
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.42	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:Q:447:TYR:CE2	5:Q:550:INO:H6	2.48	0.48
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.48	0.48
2:M:468:PRO:HD2	2:M:472:THR:HG21	1.96	0.48
1:C:78:GLU:CG	2:O:301:PRO:HG2	2.44	0.48
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.78	0.48
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.96	0.48
2:N:386:ASP:HA	2:N:527:LEU:O	2.13	0.48
2:Q:361:HIS:N	2:Q:361:HIS:CD2	2.78	0.48
1:C:80:GLN:OE1	1:C:80:GLN:HA	2.13	0.47
1:D:63:VAL:HG13	2:P:330:ARG:CZ	2.44	0.47
2:N:376:GLU:O	2:N:442:ILE:HA	2.14	0.47
2:M:516:MET:HA	2:P:448:PRO:HB2	1.96	0.47
2:O:478:LEU:HD23	2:O:478:LEU:C	2.34	0.47
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.72	0.47
1:F:18:HIS:CE1	1:F:99:PHE:CE1	3.02	0.47
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.97	0.47
2:M:326:THR:O	2:M:326:THR:CG2	2.62	0.47
2:N:488:MET:HE2	1:C:1:PRO:HG3	1.97	0.47
1:D:50:LEU:O	1:D:182:ALA:HA	2.14	0.47
1:F:74:ASP:OD1	1:F:76:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:486:ILE:N	2:N:487:PRO:HD2	2.30	0.47
2:R:392:VAL:HG21	2:R:527:LEU:HD12	1.96	0.47
2:M:522:ARG:NH1	6:M:665:HOH:O	2.44	0.47
2:O:395:THR:HG22	2:O:431:THR:CG2	2.44	0.47
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.96	0.47
1:F:124:PRO:HA	6:F:1221:HOH:O	2.15	0.47
2:P:385:VAL:O	2:P:526:VAL:HA	2.15	0.47
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.30	0.47
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.97	0.47
1:A:51:LEU:HD11	1:A:126:ILE:HD12	1.97	0.47
1:C:39:LEU:HD11	1:C:93:GLY:HA3	1.97	0.47
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.33	0.47
2:M:508:LEU:HD23	2:P:488:MET:CE	2.44	0.47
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.71	0.47
2:P:406:GLY:O	2:P:447:TYR:HD1	1.98	0.47
1:D:143:LEU:HD23	1:D:143:LEU:C	2.36	0.47
1:D:79:TYR:O	2:P:301:PRO:HB3	2.15	0.47
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.37	0.47
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.96	0.47
2:R:497:ASN:HD22	2:R:497:ASN:C	2.18	0.47
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.79	0.47
2:O:392:VAL:HG12	2:O:395:THR:HB	1.96	0.47
2:O:405:GLY:HA3	6:O:652:HOH:O	2.15	0.47
2:M:324:TYR:OH	5:M:550:INO:O1	2.25	0.46
2:M:515:PRO:HB3	2:P:453:PRO:O	2.16	0.46
2:N:399:MET:HA	2:N:462:HIS:O	2.15	0.46
2:P:497:ASN:HD22	2:P:497:ASN:C	2.18	0.46
2:Q:509:ASP:N	2:Q:520:ALA:O	2.41	0.46
2:R:416:LEU:CD2	2:R:416:LEU:C	2.83	0.46
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.98	0.46
2:N:465:ILE:HD13	2:N:525:ILE:HG21	1.97	0.46
1:B:12:THR:HA	1:B:135:ILE:O	2.16	0.46
1:B:176:GLU:OE2	1:B:179:GLY:C	2.54	0.46
1:F:143:LEU:HD23	1:F:143:LEU:C	2.36	0.46
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.51	0.46
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.97	0.46
2:P:478:LEU:C	2:P:478:LEU:HD23	2.35	0.46
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.97	0.46
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.73	0.46
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.16	0.46
2:Q:519:LEU:HA	2:Q:519:LEU:HD23	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.82	0.46
1:E:66:SER:HB2	1:E:130:LEU:HD11	1.98	0.46
1:E:180:LYS:HG2	1:E:181:THR:N	2.29	0.46
1:E:51:LEU:HD12	1:E:106:LEU:CD2	2.46	0.46
1:F:77:GLY:O	1:F:114:VAL:HG12	2.14	0.46
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.80	0.46
2:O:356:PHE:CE1	2:O:428:ARG:HD2	2.48	0.46
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.97	0.46
2:M:486:ILE:N	2:M:487:PRO:CD	2.78	0.46
2:O:434:ASP:HB3	2:O:436:TYR:CE2	2.51	0.46
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.62	0.46
1:E:13:ALA:HB2	2:Q:475:ILE:HG21	1.97	0.46
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.88	0.46
2:O:326:THR:HG22	2:O:326:THR:O	2.16	0.45
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.82	0.45
1:A:165:GLN:H	1:A:165:GLN:CD	2.20	0.45
1:F:150:GLN:O	1:F:153:ALA:HB3	2.16	0.45
1:F:35:ILE:HG21	1:F:92:PHE:CE2	2.52	0.45
1:F:74:ASP:OD1	1:F:74:ASP:C	2.54	0.45
2:O:406:GLY:O	2:O:447:TYR:HD1	1.98	0.45
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.16	0.45
2:R:384:VAL:N	2:R:435:GLY:O	2.38	0.45
1:A:50:LEU:O	1:A:182:ALA:HA	2.16	0.45
1:C:98:THR:OG1	1:C:102:GLY:N	2.49	0.45
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.45
1:E:51:LEU:HD11	1:E:126:ILE:HD12	1.98	0.45
1:F:125:HIS:HA	1:F:143:LEU:O	2.16	0.45
2:Q:415:TYR:CE1	2:Q:416:LEU:CD2	3.00	0.45
1:B:31:ARG:HD2	2:N:428:ARG:NH2	2.32	0.45
2:O:376:GLU:O	2:O:442:ILE:HA	2.17	0.45
2:O:306:SER:CB	2:O:530:GLN:HE21	2.30	0.45
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.11	0.45
2:R:434:ASP:HB3	2:R:436:TYR:HD2	1.82	0.45
1:D:19:ILE:HG22	1:D:26:ALA:HB1	1.98	0.45
1:F:54:GLN:HG3	1:F:184:ARG:HH21	1.82	0.45
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.99	0.45
2:O:395:THR:O	2:O:430:LEU:HA	2.16	0.45
2:P:400:TRP:HA	2:P:425:GLY:O	2.17	0.45
1:B:146:ASP:HB3	1:B:171:ILE:HG22	1.97	0.45
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.15	0.45
2:Q:404:ALA:HB2	2:Q:442:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG3	1:A:180:LYS:O	2.17	0.45
1:A:52:LEU:HD22	1:A:52:LEU:C	2.37	0.45
1:B:115:ASN:HA	1:B:121:PRO:HA	1.97	0.45
2:Q:449:TRP:CD1	2:Q:449:TRP:N	2.85	0.45
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.32	0.45
1:E:110:LYS:HG3	1:E:111:PRO:HD2	1.99	0.45
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.99	0.45
1:F:31:ARG:HB3	6:R:1327:HOH:O	2.16	0.45
2:P:304:ASP:OD1	2:P:307:ARG:NH1	2.48	0.45
2:R:495:ILE:HG21	2:R:500:ALA:HB3	1.99	0.45
1:D:64:ARG:CZ	1:D:100:ASP:O	2.63	0.45
1:F:33:GLN:HB3	1:F:85:LEU:HD11	1.99	0.45
2:O:395:THR:HG22	2:O:431:THR:HG23	1.98	0.45
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.51	0.44
2:O:308:PHE:CE2	2:O:530:GLN:HB2	2.52	0.44
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.99	0.44
2:Q:493:LYS:HE3	2:Q:493:LYS:HB2	1.67	0.44
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.52	0.44
1:E:52:LEU:CD2	1:E:184:ARG:HH11	2.29	0.44
1:E:87:ASN:HB3	1:E:89:PHE:O	2.17	0.44
2:P:416:LEU:CD2	2:P:416:LEU:C	2.80	0.44
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.98	0.44
1:B:50:LEU:O	1:B:182:ALA:HA	2.17	0.44
1:D:150:GLN:O	1:D:154:LYS:HG2	2.18	0.44
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.99	0.44
2:O:381:ALA:O	2:O:522:ARG:HA	2.17	0.44
2:R:350:ASN:OD1	2:R:350:ASN:C	2.55	0.44
1:E:32:ASP:HB2	6:E:265:HOH:O	2.17	0.44
1:F:48:HIS:N	1:F:48:HIS:CD2	2.85	0.44
2:M:497:ASN:ND2	2:M:499:GLU:N	2.59	0.44
2:P:315:TRP:CZ2	2:P:503:GLN:NE2	2.84	0.44
1:D:64:ARG:NE	1:D:100:ASP:O	2.50	0.44
1:B:92:PHE:CG	2:N:349:PRO:HG3	2.52	0.44
1:F:31:ARG:HH12	2:R:428:ARG:HG2	1.82	0.44
2:R:522:ARG:HH11	2:R:522:ARG:HD3	1.46	0.44
1:F:41:LYS:O	1:F:44:ALA:N	2.50	0.44
2:O:399:MET:HA	2:O:462:HIS:O	2.18	0.44
1:D:19:ILE:O	2:P:426:VAL:HG21	2.18	0.44
2:M:488:MET:CE	2:P:508:LEU:HD23	2.48	0.44
2:O:415:TYR:CE1	2:O:416:LEU:HD22	2.53	0.44
2:P:473:LYS:HD3	6:P:715:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.71	0.44
6:E:204:HOH:O	3:Q:575:CYN:C	2.66	0.44
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.53	0.44
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.47	0.44
1:F:64:ARG:HH11	1:F:64:ARG:HD2	1.29	0.44
2:O:414:ARG:HD2	2:O:414:ARG:HH11	1.62	0.44
1:F:155:CYS:HA	1:F:156:PRO:HD2	1.84	0.43
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.66	0.43
2:P:410:HIS:ND1	2:P:411:LYS:N	2.66	0.43
2:Q:363:LEU:HD11	2:Q:427:GLY:HA3	1.99	0.43
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.83	0.43
1:B:23:LEU:HD12	1:B:23:LEU:H	1.82	0.43
1:C:54:GLN:HG3	1:C:184:ARG:HH21	1.82	0.43
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.53	0.43
2:M:403:ASN:OD1	2:M:403:ASN:C	2.56	0.43
2:M:361:HIS:HB3	2:M:429:CYS:HB3	2.00	0.43
2:N:490:PRO:HA	2:N:493:LYS:HE2	2.00	0.43
2:O:364:LEU:HD22	2:O:440:ARG:CG	2.49	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.99	0.43
2:R:395:THR:HG22	2:R:431:THR:HG23	1.99	0.43
2:R:519:LEU:HA	2:R:519:LEU:HD23	1.90	0.43
1:D:19:ILE:CG2	2:P:410:HIS:HB2	2.48	0.43
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.48	0.43
2:P:522:ARG:NH1	6:P:670:HOH:O	2.48	0.43
2:M:385:VAL:O	2:M:526:VAL:HA	2.17	0.43
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.32	0.43
2:Q:536:GLU:HB2	6:Q:1096:HOH:O	2.18	0.43
2:R:306:SER:O	2:R:307:ARG:NH1	2.51	0.43
1:B:33:GLN:HG2	1:B:85:LEU:HD12	2.01	0.43
1:A:12:THR:HA	1:A:135:ILE:O	2.19	0.43
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.54	0.43
1:F:54:GLN:HG3	1:F:184:ARG:NH2	2.33	0.43
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.88	0.43
2:P:404:ALA:HB2	2:P:442:ILE:HD12	2.01	0.43
2:Q:403:ASN:HB2	6:Q:960:HOH:O	2.18	0.43
1:B:176:GLU:HA	1:B:180:LYS:O	2.18	0.43
1:B:52:LEU:HD21	1:B:184:ARG:HH12	1.83	0.43
1:C:12:THR:HA	1:C:135:ILE:O	2.19	0.43
1:E:38:ARG:HG3	1:E:107:HIS:HB2	1.99	0.43
2:Q:497:ASN:C	2:Q:497:ASN:HD22	2.22	0.43
1:E:54:GLN:OE1	1:E:184:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:361:HIS:CD2	2:O:361:HIS:N	2.79	0.43
2:P:364:LEU:HB2	2:P:440:ARG:HD3	2.00	0.43
2:Q:447:TYR:CD2	5:Q:550:INO:H6	2.53	0.43
1:B:2:ILE:O	1:B:3:GLU:OE1	2.37	0.43
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.53	0.43
1:A:157:VAL:O	1:A:160:LEU:HB2	2.19	0.42
1:C:15:PRO:HB3	1:C:133:ARG:HD2	2.01	0.42
1:E:108:THR:OG1	1:E:109:VAL:N	2.49	0.42
2:Q:362:ASP:OD1	2:Q:364:LEU:HB2	2.19	0.42
2:R:465:ILE:N	2:R:465:ILE:HD12	2.33	0.42
1:C:126:ILE:HD12	1:C:143:LEU:HD22	2.01	0.42
1:E:74:ASP:N	1:E:78:GLU:O	2.41	0.42
2:N:364:LEU:HB2	2:N:440:ARG:HD3	2.01	0.42
2:N:493:LYS:HB2	2:N:493:LYS:HE2	1.83	0.42
2:P:373:PRO:HB3	2:P:423:PHE:HB2	2.00	0.42
2:N:307:ARG:HA	2:N:307:ARG:HD3	1.83	0.42
2:N:363:LEU:N	2:N:363:LEU:HD12	2.34	0.42
2:N:511:ASN:OD1	6:N:742:HOH:O	2.21	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:131:PHE:CE2	1:E:138:HIS:HB3	2.54	0.42
1:F:143:LEU:HD23	1:F:144:TYR:N	2.34	0.42
1:E:52:LEU:HD22	1:E:52:LEU:C	2.39	0.42
1:F:64:ARG:HD3	1:F:99:PHE:O	2.19	0.42
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.84	0.42
2:P:304:ASP:CG	2:P:307:ARG:HH12	2.22	0.42
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	2.01	0.42
1:A:24:GLU:O	1:A:27:GLY:N	2.46	0.42
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.02	0.42
2:P:394:ASN:HA	2:P:431:THR:O	2.20	0.42
1:E:170:LEU:HD21	1:E:196:VAL:HB	2.01	0.42
1:F:44:ALA:HA	1:F:45:PRO:HD2	1.81	0.42
2:N:371:GLY:HA3	2:N:422:ASN:ND2	2.35	0.42
2:Q:350:ASN:C	2:Q:350:ASN:OD1	2.57	0.42
1:E:19:ILE:CG2	2:Q:410:HIS:HB2	2.50	0.42
1:C:116:ASN:C	1:C:116:ASN:OD1	2.58	0.42
2:M:519:LEU:HD23	2:M:519:LEU:HA	1.85	0.42
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.83	0.42
1:F:40:ALA:HB2	1:F:89:PHE:HD2	1.84	0.42
2:Q:487:PRO:O	2:Q:493:LYS:HD3	2.20	0.42
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:HA	1:C:36:TRP:CE3	2.53	0.42
1:F:32:ASP:HB2	6:R:1378:HOH:O	2.19	0.42
1:F:52:LEU:HD22	1:F:52:LEU:C	2.40	0.42
1:B:63:VAL:HG13	2:N:330:ARG:CZ	2.50	0.42
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.71	0.42
2:Q:395:THR:O	2:Q:430:LEU:HA	2.20	0.42
2:Q:395:THR:HG22	2:Q:431:THR:HG23	2.01	0.42
2:R:307:ARG:CG	2:R:533:THR:HG22	2.49	0.42
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.98	0.41
1:C:52:LEU:HA	1:C:104:TRP:O	2.20	0.41
1:D:51:LEU:HD12	1:D:106:LEU:HD23	2.02	0.41
1:E:31:ARG:O	1:E:32:ASP:C	2.58	0.41
2:O:536:GLU:HB2	6:O:704:HOH:O	2.18	0.41
2:P:484:PRO:O	2:P:487:PRO:HD2	2.20	0.41
2:R:484:PRO:O	2:R:487:PRO:HD2	2.20	0.41
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.84	0.41
1:A:63:VAL:HG13	2:M:330:ARG:CZ	2.50	0.41
1:F:200:PHE:CG	2:R:345:GLU:HG2	2.56	0.41
1:E:38:ARG:HH11	1:E:38:ARG:HD2	1.66	0.41
2:M:450:ARG:HG3	6:M:632:HOH:O	2.19	0.41
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.20	0.41
2:R:321:THR:HG21	2:R:494:SER:HB2	2.01	0.41
1:A:191:GLY:O	1:A:194:GLU:HB2	2.20	0.41
1:E:114:VAL:HG23	1:E:122:MET:HE2	2.01	0.41
1:E:39:LEU:O	1:E:89:PHE:HA	2.20	0.41
1:F:81:ASP:HB2	2:R:348:GLY:O	2.21	0.41
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.50	0.41
2:R:395:THR:HG22	2:R:431:THR:HG21	2.02	0.41
1:C:52:LEU:HD22	1:C:52:LEU:C	2.41	0.41
1:C:18:HIS:CE1	1:C:99:PHE:CE1	3.09	0.41
1:D:65:ASP:OD2	1:D:133:ARG:CD	2.68	0.41
2:P:381:ALA:HB2	2:P:438:SER:HB2	2.02	0.41
2:P:420:ASP:HA	2:P:421:PRO:HD2	1.96	0.41
1:D:131:PHE:O	1:D:132:ALA:HB2	2.21	0.41
1:E:15:PRO:HB3	1:E:133:ARG:HD2	2.03	0.41
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.55	0.41
2:R:485:LEU:HA	2:R:485:LEU:HD23	1.92	0.41
1:C:19:ILE:CG1	2:O:400:TRP:HB2	2.50	0.41
1:D:39:LEU:HB3	1:D:90:ASN:O	2.20	0.41
1:F:33:GLN:HG2	1:F:85:LEU:CD1	2.48	0.41
2:N:447:TYR:HA	2:N:448:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LEU:HD12	1:C:51:LEU:H	1.84	0.41
1:D:39:LEU:HD12	1:D:39:LEU:N	2.34	0.41
1:E:51:LEU:HB2	1:E:106:LEU:HB3	2.02	0.41
1:E:36:TRP:CG	1:E:37:ASN:N	2.87	0.41
2:R:372:LEU:HA	2:R:372:LEU:HD12	1.82	0.41
1:A:180:LYS:HG2	1:A:181:THR:N	2.34	0.41
1:A:64:ARG:HD2	1:A:64:ARG:HH11	1.66	0.41
1:A:9:PRO:HG3	2:M:500:ALA:HB1	2.03	0.41
1:C:26:ALA:O	2:O:411:LYS:HG3	2.21	0.41
1:C:18:HIS:CE1	1:C:99:PHE:HE1	2.39	0.41
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.50	0.41
1:F:154:LYS:HA	1:F:154:LYS:HD2	1.55	0.41
2:M:473:LYS:HD2	2:M:474:LEU:H	1.86	0.41
2:O:410:HIS:CE1	2:O:412:ASN:H	2.39	0.41
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.84	0.41
1:A:199:ASP:CG	2:M:313:ARG:HE	2.23	0.41
1:C:19:ILE:HG13	2:O:426:VAL:HG22	2.02	0.41
2:M:409:ARG:NH2	2:M:420:ASP:O	2.51	0.41
2:M:448:PRO:CB	2:P:516:MET:HA	2.50	0.41
2:Q:360:ASP:O	2:Q:427:GLY:HA2	2.21	0.41
2:Q:468:PRO:HD2	2:Q:472:THR:HG21	2.03	0.41
1:A:98:THR:O	1:A:102:GLY:HA2	2.21	0.41
1:A:66:SER:HA	1:A:132:ALA:HB2	2.02	0.41
1:B:31:ARG:HB3	6:N:699:HOH:O	2.21	0.41
1:E:51:LEU:O	1:E:105:THR:HA	2.20	0.41
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.86	0.41
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.74	0.40
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.89	0.40
2:N:465:ILE:CD1	2:N:525:ILE:HD13	2.51	0.40
2:P:489:CYS:O	2:P:493:LYS:HE3	2.21	0.40
2:Q:450:ARG:HH11	2:Q:450:ARG:HD2	1.64	0.40
1:C:66:SER:HA	1:C:132:ALA:HB2	2.04	0.40
1:D:61:HIS:HD1	1:E:163:GLN:HG3	1.86	0.40
1:F:100:ASP:N	1:F:100:ASP:OD1	2.53	0.40
2:Q:447:TYR:HA	2:Q:448:PRO:HD3	1.99	0.40
2:R:306:SER:HB3	2:R:530:GLN:HE21	1.84	0.40
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.21	0.40
2:M:376:GLU:OE1	2:M:443:LYS:HD3	2.21	0.40
1:B:191:GLY:O	1:B:194:GLU:HB2	2.22	0.40
1:D:131:PHE:CE1	1:D:138:HIS:CB	3.04	0.40
1:D:176:GLU:HG3	1:D:180:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG2	2:M:301:PRO:HG3	2.02	0.40
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.73	0.40
2:R:447:TYR:HA	2:R:448:PRO:HD3	1.95	0.40
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	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%)	32	25
1	D	198/200 (99%)	188 (95%)	9 (4%)	1 (0%)	32	25
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	32	25
2	M	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	N	229/238 (96%)	222 (97%)	6 (3%)	1 (0%)	38	32
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	8 (4%)	1 (0%)	38	32
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	10 (4%)	1 (0%)	38	32
All	All	2562/2628 (98%)	2445 (95%)	111 (4%)	6 (0%)	51	50

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%)	154 (95%)	8 (5%)	29	24
1	B	162/163 (99%)	153 (94%)	9 (6%)	25	19
1	C	162/163 (99%)	155 (96%)	7 (4%)	33	30
1	D	162/163 (99%)	153 (94%)	9 (6%)	25	19
1	E	162/163 (99%)	157 (97%)	5 (3%)	45	44
1	F	162/163 (99%)	155 (96%)	7 (4%)	33	30
2	M	196/202 (97%)	188 (96%)	8 (4%)	35	33
2	N	196/202 (97%)	189 (96%)	7 (4%)	40	38
2	O	196/202 (97%)	183 (93%)	13 (7%)	19	13
2	P	196/202 (97%)	187 (95%)	9 (5%)	31	27
2	Q	196/202 (97%)	184 (94%)	12 (6%)	22	16
2	R	196/202 (97%)	183 (93%)	13 (7%)	19	13
All	All	2148/2190 (98%)	2041 (95%)	107 (5%)	28	23

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	24	GLU
1	A	38	ARG
1	A	52	LEU
1	A	100	ASP

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Mol	Chain	Res	Type
1	A	164	PRO
1	A	165	GLN
1	A	184	ARG
2	M	364	LEU
2	M	395	THR
2	M	416	LEU
2	M	434	ASP
2	M	440	ARG
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	9	PRO
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	91	SER
1	B	133	ARG
1	B	165	GLN
1	B	176	GLU
2	N	364	LEU
2	N	395	THR
2	N	416	LEU
2	N	429	CYS
2	N	440	ARG
2	N	497	ASN
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	66	SER
1	C	158	LEU
1	C	165	GLN
2	O	372	LEU
2	O	395	THR
2	O	399	MET
2	O	414	ARG
2	O	416	LEU
2	O	428	ARG
2	O	429	CYS
2	O	434	ASP

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Mol	Chain	Res	Type
2	O	438	SER
2	O	440	ARG
2	O	497	ASN
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	114	VAL
1	D	165	GLN
1	D	184	ARG
2	P	395	THR
2	P	399	MET
2	P	416	LEU
2	P	429	CYS
2	P	434	ASP
2	P	438	SER
2	P	440	ARG
2	P	497	ASN
2	P	534	HIS
1	E	19	ILE
1	E	52	LEU
1	E	100	ASP
1	E	165	GLN
1	E	181	THR
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	434	ASP
2	Q	440	ARG
2	Q	473	LYS
2	Q	497	ASN
2	Q	503	GLN
2	Q	507	LYS
1	F	4	LEU
1	F	42	PRO

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Mol	Chain	Res	Type
1	F	50	LEU
1	F	52	LEU
1	F	94	ARG
1	F	100	ASP
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	497	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

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

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Mol	Chain	Res	Type
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	422	ASN
2	Q	497	ASN
2	Q	503	GLN
1	F	18	HIS
1	F	80	GLN
1	F	159	ASN
1	F	165	GLN
2	R	361	HIS
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	INO	M	550	4	5,11,11	1.58	1 (20%)	5,15,15	0.83	0
3	CYN	M	575	4	0,1,1	0.00	-	0,0,0	0.00	-
5	INO	N	550	4	5,11,11	1.42	1 (20%)	5,15,15	0.73	0
3	CYN	N	575	4	0,1,1	0.00	-	0,0,0	0.00	-
5	INO	O	550	4	5,11,11	1.44	1 (20%)	5,15,15	0.92	0
3	CYN	O	575	4	0,1,1	0.00	-	0,0,0	0.00	-
5	INO	P	550	4	5,11,11	1.39	1 (20%)	5,15,15	0.55	0
3	CYN	P	575	4	0,1,1	0.00	-	0,0,0	0.00	-
5	INO	Q	550	4	5,11,11	1.31	1 (20%)	5,15,15	0.58	0
3	CYN	Q	575	4	0,1,1	0.00	-	0,0,0	0.00	-
5	INO	R	550	4	5,11,11	1.27	1 (20%)	5,15,15	0.60	0
3	CYN	R	575	4	0,1,1	0.00	-	0,0,0	0.00	-

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	M	550	4	-	0/0/4/4	0/1/1/1
3	CYN	M	575	4	-	0/0/0/0	0/0/0/0
5	INO	N	550	4	-	0/0/4/4	0/1/1/1
3	CYN	N	575	4	-	0/0/0/0	0/0/0/0
5	INO	O	550	4	-	0/0/4/4	0/1/1/1
3	CYN	O	575	4	-	0/0/0/0	0/0/0/0
5	INO	P	550	4	-	0/0/4/4	0/1/1/1
3	CYN	P	575	4	-	0/0/0/0	0/0/0/0
5	INO	Q	550	4	-	0/0/4/4	0/1/1/1
3	CYN	Q	575	4	-	0/0/0/0	0/0/0/0
5	INO	R	550	4	-	0/0/4/4	0/1/1/1
3	CYN	R	575	4	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	550	INO	O3-C2	-3.05	1.23	1.32
5	N	550	INO	O3-C2	-2.59	1.25	1.32
5	Q	550	INO	O3-C2	-2.48	1.25	1.32
5	O	550	INO	O3-C2	-2.46	1.25	1.32
5	P	550	INO	O3-C2	-2.38	1.25	1.32
5	R	550	INO	O3-C2	-2.09	1.26	1.32

There are no bond angle outliers.

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	O	575	CYN	1	0
3	P	575	CYN	1	0
5	Q	550	INO	2	0
3	Q	575	CYN	2	0
3	R	575	CYN	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.