



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:45 am BST

PDB ID : 2PCD
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE FROM
PSEUDOMONAS AERUGINOSA AT 2.15 ANGSTROMS RESOLUTION
Authors : Ohlendorf, D.H.; Orville, A.M.; Lipscomb, J.D.
Deposited on : 1994-06-21
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

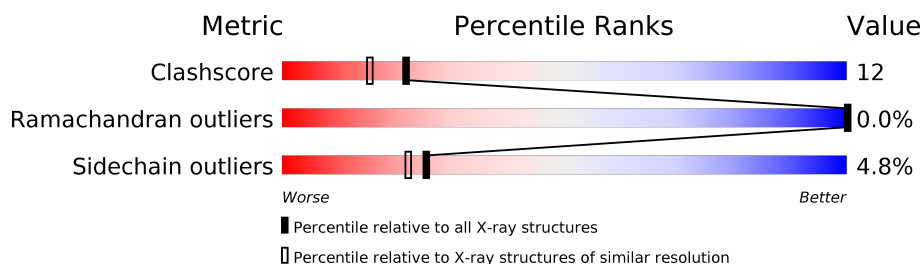
1 Overall quality at a glance

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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (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 ≥ 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	75% 19% 5% •
1	B	200	73% 21% 7%
1	C	200	72% 23% 5% •
1	D	200	74% 21% 5%
1	E	200	72% 25% • •
1	F	200	68% 27% • •
2	M	238	74% 21% • • •
2	N	238	78% 15% 5% •

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Mol	Chain	Length	Quality of chain
2	O	238	<div><div></div><div>73%20%</div><div></div><div></div></div>
2	P	238	<div><div></div><div>74%19%</div><div></div><div></div></div>
2	Q	238	<div><div></div><div>69%24%5%</div><div></div><div></div></div>
2	R	238	<div><div></div><div>66%27%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 (BETA CHAIN).

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

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is water.

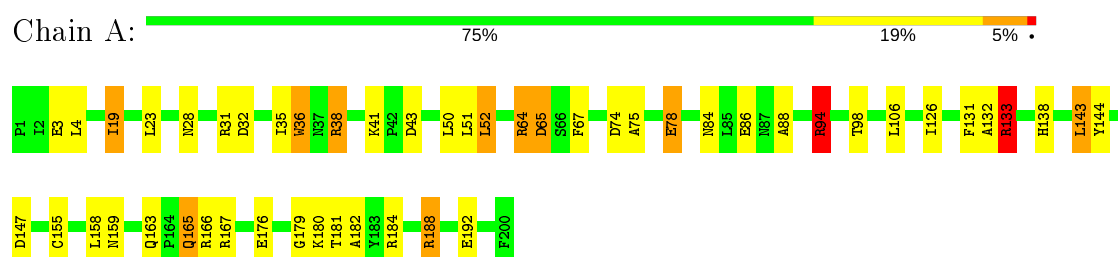
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	M	154	Total O 154 154	0	0
4	B	79	Total O 79 79	0	0
4	N	163	Total O 163 163	0	0
4	C	80	Total O 80 80	0	0
4	O	158	Total O 158 158	0	0
4	D	77	Total O 77 77	0	0
4	P	159	Total O 159 159	0	0
4	E	77	Total O 77 77	0	0
4	Q	163	Total O 163 163	0	0
4	F	83	Total O 83 83	0	0
4	R	158	Total O 158 158	0	0

3 Residue-property plots [i](#)

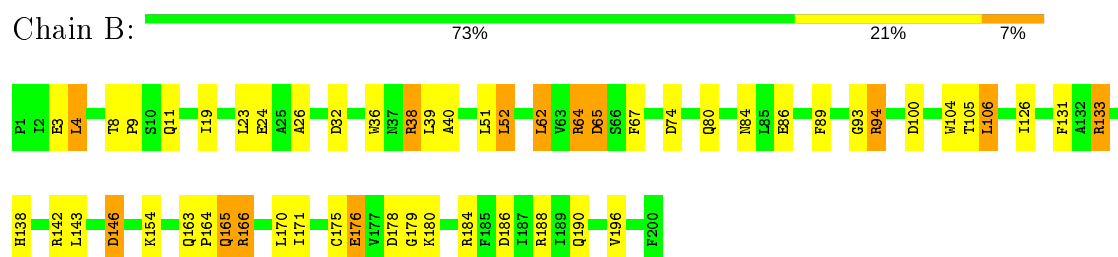
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

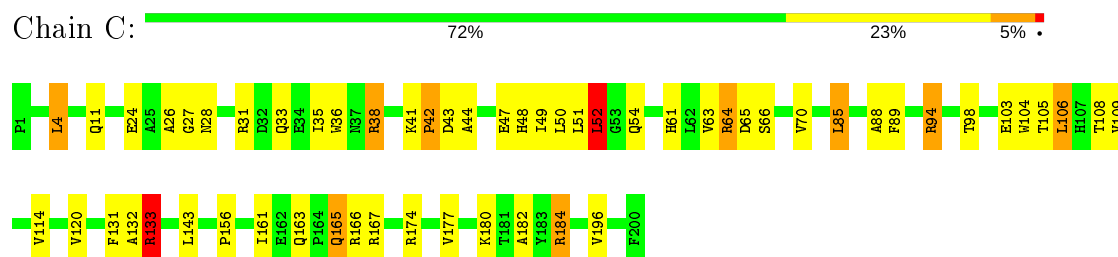
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)



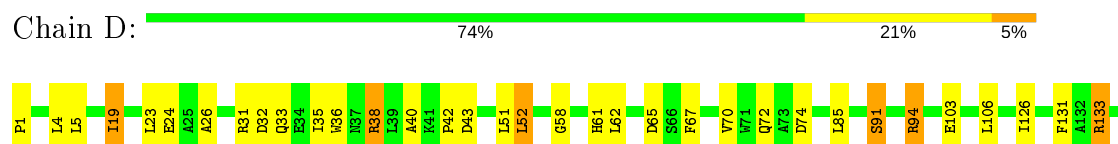
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

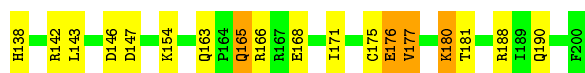


• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)



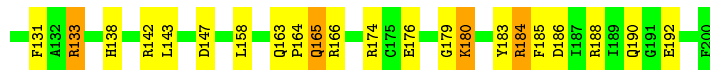
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)





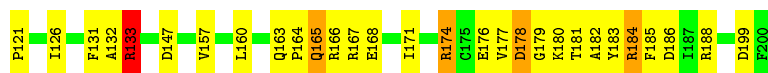
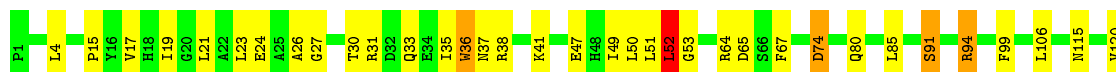
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain E: 72% 25% . .



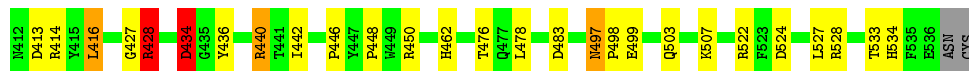
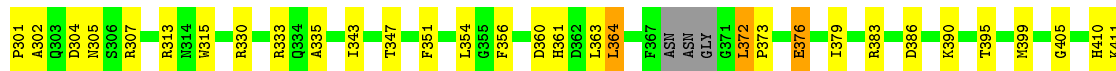
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE (ALPHA CHAIN)

Chain F: 68% 27% . .



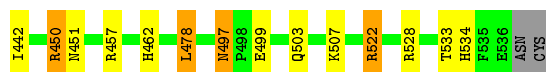
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

Chain M: 74% 21% . . .



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

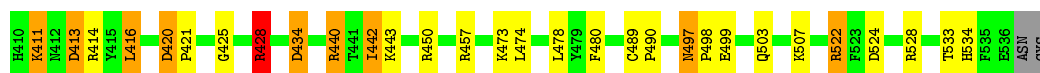
Chain N: 78% 15% 5% .



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

Chain O: 73% 20% . .





- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

Chain P: 74% 19%



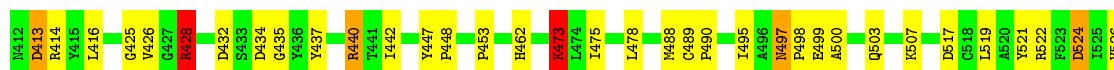
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

Chain Q: 69% 24% 5%



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE (BETA CHAIN)

Chain R: 66% 27% 7%



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	197.17Å 127.03Å 134.18Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	5.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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

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	0.99	1/1611 (0.1%)	1.72	32/2195 (1.5%)
1	B	0.98	1/1611 (0.1%)	1.61	29/2195 (1.3%)
1	C	1.00	0/1611	1.64	22/2195 (1.0%)
1	D	0.99	1/1611 (0.1%)	1.73	32/2195 (1.5%)
1	E	1.02	0/1611	1.72	27/2195 (1.2%)
1	F	1.06	0/1611	1.72	28/2195 (1.3%)
2	M	1.00	1/1895 (0.1%)	1.63	26/2580 (1.0%)
2	N	1.02	1/1895 (0.1%)	1.66	33/2580 (1.3%)
2	O	1.01	0/1895	1.60	34/2580 (1.3%)
2	P	1.01	2/1895 (0.1%)	1.57	25/2580 (1.0%)
2	Q	1.08	1/1895 (0.1%)	1.63	35/2580 (1.4%)
2	R	1.07	0/1895	1.65	32/2580 (1.2%)
All	All	1.02	8/21036 (0.0%)	1.66	355/28650 (1.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-5.99	1.36	1.46
2	P	428	ARG	CD-NE	-5.71	1.36	1.46
2	N	440	ARG	CD-NE	-5.67	1.36	1.46
1	B	94	ARG	CD-NE	-5.65	1.36	1.46
2	P	345	GLU	CD-OE1	-5.59	1.19	1.25
1	D	94	ARG	CD-NE	-5.59	1.36	1.46
2	Q	367	PHE	C-O	5.17	1.33	1.23
2	M	428	ARG	CD-NE	-5.01	1.38	1.46

All (355) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	440	ARG	NE-CZ-NH2	-24.05	108.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	440	ARG	NE-CZ-NH2	-23.06	108.77	120.30
2	Q	440	ARG	NE-CZ-NH2	-22.31	109.14	120.30
2	R	440	ARG	NE-CZ-NH2	-20.05	110.28	120.30
1	F	38	ARG	CD-NE-CZ	19.67	151.13	123.60
2	P	440	ARG	NE-CZ-NH2	-18.56	111.02	120.30
1	E	133	ARG	NE-CZ-NH1	18.08	129.34	120.30
2	O	440	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	C	133	ARG	NE-CZ-NH1	17.14	128.87	120.30
1	A	94	ARG	CD-NE-CZ	17.03	147.44	123.60
1	D	94	ARG	NE-CZ-NH2	-16.46	112.07	120.30
1	A	133	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	D	94	ARG	NE-CZ-NH1	14.13	127.37	120.30
2	M	450	ARG	NE-CZ-NH1	13.89	127.25	120.30
2	P	440	ARG	NE-CZ-NH1	13.69	127.15	120.30
1	B	184	ARG	NE-CZ-NH2	-13.51	113.55	120.30
1	E	133	ARG	CD-NE-CZ	13.51	142.51	123.60
1	D	166	ARG	NE-CZ-NH1	13.35	126.97	120.30
2	N	440	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	F	38	ARG	NE-CZ-NH1	13.11	126.86	120.30
1	D	94	ARG	CD-NE-CZ	13.04	141.86	123.60
1	C	94	ARG	CD-NE-CZ	13.04	141.85	123.60
1	E	38	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	D	166	ARG	NE-CZ-NH2	-12.73	113.94	120.30
2	M	313	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	E	64	ARG	NE-CZ-NH1	12.39	126.49	120.30
1	C	94	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	B	38	ARG	NE-CZ-NH2	-12.15	114.22	120.30
2	N	307	ARG	NE-CZ-NH1	12.11	126.35	120.30
2	Q	522	ARG	NE-CZ-NH1	-12.04	114.28	120.30
2	R	407	ARG	NE-CZ-NH1	11.96	126.28	120.30
2	R	407	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	F	31	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	A	31	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	D	188	ARG	NE-CZ-NH1	11.65	126.12	120.30
2	N	428	ARG	NE-CZ-NH2	-11.63	114.48	120.30
2	Q	311	ARG	NE-CZ-NH2	-11.59	114.50	120.30
2	Q	311	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	Q	428	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	A	94	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	A	184	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	D	65	ASP	CB-CG-OD1	11.20	128.38	118.30
1	E	133	ARG	NE-CZ-NH2	-11.16	114.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	94	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	F	94	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	133	ARG	CD-NE-CZ	10.87	138.81	123.60
2	N	330	ARG	NE-CZ-NH2	-10.83	114.88	120.30
1	E	52	LEU	CA-CB-CG	10.78	140.08	115.30
1	A	64	ARG	NE-CZ-NH1	-10.77	114.92	120.30
1	E	64	ARG	NE-CZ-NH2	-10.61	114.99	120.30
1	A	188	ARG	NE-CZ-NH1	10.51	125.56	120.30
2	P	428	ARG	NE-CZ-NH1	10.45	125.53	120.30
2	P	524	ASP	CB-CG-OD1	10.44	127.70	118.30
2	N	333	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	D	133	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	31	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	94	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	D	38	ARG	NE-CZ-NH2	-10.17	115.21	120.30
2	O	330	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	Q	457	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	B	186	ASP	CB-CG-OD1	10.01	127.31	118.30
1	F	38	ARG	CA-CB-CG	9.97	135.34	113.40
1	F	174	ARG	NE-CZ-NH2	-9.91	115.34	120.30
1	D	133	ARG	CD-NE-CZ	9.86	137.40	123.60
2	M	428	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	E	184	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	M	383	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	F	167	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	C	166	ARG	NE-CZ-NH1	9.72	125.16	120.30
2	N	457	ARG	NE-CZ-NH2	-9.66	115.47	120.30
2	Q	440	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	F	166	ARG	NE-CZ-NH1	9.62	125.11	120.30
2	M	434	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	A	65	ASP	CB-CG-OD1	9.43	126.79	118.30
2	Q	428	ARG	NE-CZ-NH1	9.33	124.97	120.30
2	M	428	ARG	NE-CZ-NH1	9.24	124.92	120.30
2	N	414	ARG	NE-CZ-NH2	-9.24	115.68	120.30
2	O	377	ARG	NE-CZ-NH1	9.22	124.91	120.30
2	O	428	ARG	NE-CZ-NH1	9.18	124.89	120.30
2	O	428	ARG	CD-NE-CZ	9.15	136.41	123.60
1	B	94	ARG	CG-CD-NE	9.03	130.77	111.80
1	B	166	ARG	NE-CZ-NH1	9.02	124.81	120.30
2	O	409	ARG	NE-CZ-NH2	8.93	124.77	120.30
1	E	184	ARG	NE-CZ-NH2	-8.93	115.83	120.30
2	R	524	ASP	CB-CG-OD1	8.93	126.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	D	133	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	R	362	ASP	CB-CG-OD2	8.80	126.22	118.30
1	E	166	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	R	307	ARG	NE-CZ-NH1	8.77	124.69	120.30
2	R	409	ARG	NE-CZ-NH1	8.73	124.66	120.30
2	R	432	ASP	CB-CG-OD2	-8.71	110.46	118.30
2	R	383	ARG	NE-CZ-NH2	-8.71	115.95	120.30
2	N	311	ARG	NE-CZ-NH2	-8.57	116.01	120.30
2	O	313	ARG	NE-CZ-NH1	8.56	124.58	120.30
2	M	450	ARG	NE-CZ-NH2	-8.51	116.05	120.30
2	N	313	ARG	NE-CZ-NH1	8.47	124.54	120.30
2	Q	377	ARG	NE-CZ-NH1	-8.43	116.08	120.30
2	M	428	ARG	CD-NE-CZ	8.43	135.40	123.60
2	O	428	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	E	142	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	52	LEU	CB-CA-C	8.38	126.12	110.20
1	E	186	ASP	CB-CG-OD1	8.38	125.84	118.30
1	E	94	ARG	NE-CZ-NH1	8.31	124.45	120.30
2	M	524	ASP	CB-CG-OD1	8.28	125.75	118.30
2	P	383	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	P	428	ARG	CG-CD-NE	8.24	129.12	111.80
1	D	38	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	D	36	TRP	CB-CA-C	8.18	126.76	110.40
1	B	133	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	C	133	ARG	CD-NE-CZ	8.08	134.91	123.60
2	R	440	ARG	NE-CZ-NH1	8.05	124.32	120.30
2	P	428	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	31	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	D	65	ASP	CB-CG-OD2	-8.02	111.08	118.30
2	M	313	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	N	434	ASP	CB-CG-OD2	-7.91	111.18	118.30
2	N	307	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	P	524	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	F	186	ASP	CB-CG-OD1	7.87	125.39	118.30
1	C	184	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	P	428	ARG	CD-NE-CZ	7.79	134.51	123.60
1	B	184	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	94	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	F	52	LEU	CB-CA-C	7.72	124.86	110.20
2	O	330	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	94	ARG	CA-CB-CG	7.61	130.14	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	434	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	E	94	ARG	NE-CZ-NH2	-7.58	116.51	120.30
2	R	383	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	F	188	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	64	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	O	528	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	F	65	ASP	CB-CG-OD1	7.42	124.98	118.30
2	N	383	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	24	GLU	CA-CB-CG	7.38	129.64	113.40
1	C	106	LEU	CA-CB-CG	7.37	132.26	115.30
2	R	383	ARG	NH1-CZ-NH2	7.37	127.51	119.40
2	N	457	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	52	LEU	CB-CA-C	7.34	124.14	110.20
1	C	52	LEU	CB-CA-C	7.32	124.11	110.20
2	P	307	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	P	457	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	Q	383	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	188	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	133	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	166	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	Q	432	ASP	CB-CG-OD1	7.10	124.69	118.30
2	P	333	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	F	74	ASP	CB-CG-OD1	7.03	124.63	118.30
2	M	440	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	78	GLU	OE1-CD-OE2	6.96	131.65	123.30
2	Q	440	ARG	CD-NE-CZ	6.90	133.26	123.60
1	F	38	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	184	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	64	ARG	CD-NE-CZ	-6.81	114.07	123.60
2	Q	311	ARG	CD-NE-CZ	6.81	133.13	123.60
1	B	178	ASP	CB-CG-OD1	6.80	124.42	118.30
2	O	450	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	64	ARG	NE-CZ-NH2	-6.75	116.92	120.30
2	P	434	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	E	186	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	E	174	ARG	NE-CZ-NH1	-6.74	116.93	120.30
2	M	383	ARG	NH1-CZ-NH2	6.74	126.81	119.40
2	O	377	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	N	416	LEU	CB-CA-C	6.72	122.98	110.20
2	Q	376	GLU	OE1-CD-OE2	6.70	131.33	123.30
2	Q	524	ASP	CB-CG-OD1	6.69	124.32	118.30
2	O	383	ARG	NE-CZ-NH2	-6.69	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	457	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	174	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	F	31	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	75	ALA	CB-CA-C	6.64	120.06	110.10
2	N	414	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	133	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	142	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	11	GLN	N-CA-CB	6.57	122.43	110.60
1	C	94	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	M	330	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	167	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	166	ARG	NE-CZ-NH2	-6.51	117.04	120.30
2	N	333	ARG	CD-NE-CZ	-6.50	114.50	123.60
2	Q	457	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	36	TRP	CB-CA-C	6.49	123.37	110.40
2	O	333	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	147	ASP	CB-CG-OD1	6.47	124.13	118.30
2	O	407	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	O	440	ARG	NH1-CZ-NH2	6.46	126.50	119.40
2	N	312	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	176	GLU	OE1-CD-OE2	-6.37	115.66	123.30
1	B	38	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	52	LEU	CA-CB-CG	6.36	129.93	115.30
2	R	473	LYS	CA-CB-CG	6.35	127.38	113.40
1	B	65	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	147	ASP	CB-CG-OD1	6.33	124.00	118.30
2	N	416	LEU	CA-CB-CG	6.33	129.85	115.30
2	M	354	LEU	CB-CA-C	6.29	122.16	110.20
1	B	94	ARG	CB-CG-CD	6.29	127.96	111.60
2	P	455	ASP	CB-CG-OD1	6.29	123.96	118.30
1	F	64	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	M	440	ARG	NH1-CZ-NH2	6.24	126.27	119.40
2	R	536	GLU	CG-CD-OE1	6.24	130.78	118.30
2	O	409	ARG	NE-CZ-NH1	-6.24	117.18	120.30
2	M	528	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	74	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	N	528	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	N	333	ARG	NH1-CZ-NH2	6.16	126.18	119.40
2	R	517	ASP	CB-CG-OD1	6.16	123.84	118.30
2	R	428	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	E	31	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	R	323	ASP	CB-CG-OD1	6.14	123.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	GLU	CA-CB-CG	6.13	126.89	113.40
1	F	64	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	O	353	HIS	CA-CB-CG	-6.11	103.22	113.60
2	Q	409	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	43	ASP	CB-CG-OD2	-6.07	112.83	118.30
2	R	383	ARG	N-CA-CB	-6.06	99.69	110.60
2	O	416	LEU	CB-CA-C	6.04	121.68	110.20
1	A	65	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	74	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	175	CYS	CA-CB-SG	6.01	124.82	114.00
2	Q	383	ARG	CD-NE-CZ	-6.00	115.19	123.60
2	R	428	ARG	CG-CD-NE	6.00	124.41	111.80
1	D	175	CYS	CA-CB-SG	6.00	124.80	114.00
1	A	23	LEU	CB-CA-C	5.96	121.53	110.20
2	N	522	ARG	CD-NE-CZ	5.96	131.94	123.60
2	Q	307	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	N	434	ASP	CA-CB-CG	-5.96	100.30	113.40
2	M	434	ASP	OD1-CG-OD2	5.95	134.61	123.30
1	F	133	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	M	434	ASP	CA-CB-CG	-5.93	100.36	113.40
1	C	52	LEU	CA-CB-CG	5.92	128.93	115.30
1	A	32	ASP	CB-CG-OD1	5.91	123.62	118.30
1	F	199	ASP	CB-CG-OD1	5.91	123.62	118.30
2	P	372	LEU	CB-CA-C	5.89	121.39	110.20
2	N	528	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	146	ASP	CB-CG-OD1	5.88	123.59	118.30
2	O	457	ARG	CA-CB-CG	5.88	126.33	113.40
1	E	166	ARG	NE-CZ-NH2	-5.87	117.37	120.30
2	Q	313	ARG	NE-CZ-NH2	5.81	123.20	120.30
2	Q	372	LEU	N-CA-CB	-5.79	98.83	110.40
2	O	528	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	P	483	ASP	CB-CG-OD2	5.75	123.47	118.30
2	N	450	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	32	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	O	428	ARG	CB-CG-CD	5.73	126.51	111.60
1	B	38	ARG	CD-NE-CZ	5.72	131.61	123.60
1	F	106	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	167	ARG	CD-NE-CZ	-5.71	115.60	123.60
2	P	333	ARG	CD-NE-CZ	-5.71	115.61	123.60
2	P	416	LEU	CA-CB-CG	5.70	128.40	115.30
2	R	413	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	147	ASP	CB-CG-OD2	-5.68	113.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	377	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	C	36	TRP	CB-CA-C	5.65	121.70	110.40
1	D	23	LEU	CB-CA-C	5.63	120.91	110.20
1	A	166	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	M	428	ARG	CG-CD-NE	5.60	123.56	111.80
1	E	36	TRP	CB-CA-C	5.59	121.58	110.40
2	Q	522	ARG	CD-NE-CZ	-5.58	115.78	123.60
2	Q	474	LEU	N-CA-CB	-5.58	99.25	110.40
2	O	420	ASP	CB-CG-OD1	5.57	123.32	118.30
2	O	413	ASP	CB-CG-OD1	5.57	123.31	118.30
2	M	333	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	Q	434	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	M	483	ASP	CB-CG-OD2	5.53	123.28	118.30
2	O	522	ARG	NE-CZ-NH1	-5.53	117.54	120.30
2	Q	312	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	24	GLU	OE1-CD-OE2	5.51	129.91	123.30
2	Q	432	ASP	CB-CG-OD2	-5.50	113.34	118.30
1	C	38	ARG	CD-NE-CZ	-5.50	115.90	123.60
2	P	313	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	11	GLN	N-CA-CB	5.49	120.48	110.60
2	N	428	ARG	CG-CD-NE	5.47	123.30	111.80
2	O	416	LEU	CA-CB-CG	5.47	127.89	115.30
2	O	323	ASP	CB-CG-OD1	5.46	123.21	118.30
1	E	86	GLU	CG-CD-OE1	5.46	129.21	118.30
2	N	434	ASP	OD1-CG-OD2	5.45	133.66	123.30
2	Q	440	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	D	103	GLU	CG-CD-OE1	-5.44	107.41	118.30
2	Q	367	PHE	CA-C-O	-5.43	108.69	120.10
2	Q	413	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	100	ASP	CB-CG-OD2	-5.40	113.44	118.30
2	R	440	ARG	NH1-CZ-NH2	5.38	125.31	119.40
2	M	476	THR	CA-CB-CG2	5.37	119.92	112.40
2	N	440	ARG	CB-CG-CD	-5.36	97.67	111.60
1	D	62	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	52	LEU	CB-CA-C	5.35	120.36	110.20
2	R	361	HIS	CA-CB-CG	-5.34	104.53	113.60
1	F	36	TRP	CB-CA-C	5.33	121.05	110.40
2	M	383	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	R	353	HIS	CA-CB-CG	-5.32	104.55	113.60
1	C	94	ARG	CB-CG-CD	5.32	125.42	111.60
1	F	52	LEU	CA-CB-CG	5.30	127.48	115.30
1	D	31	ARG	NE-CZ-NH2	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	O	457	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	176	GLU	CA-CB-CG	5.27	125.00	113.40
2	Q	360	ASP	CB-CG-OD2	-5.27	113.56	118.30
2	N	428	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	Q	383	ARG	NH1-CZ-NH2	5.25	125.18	119.40
2	P	432	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	184	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	F	184	ARG	CD-NE-CZ	-5.25	116.26	123.60
1	E	68	LEU	CA-CB-CG	5.24	127.35	115.30
2	P	377	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	E	183	TYR	CA-CB-CG	5.21	123.30	113.40
2	Q	416	LEU	CB-CA-C	5.21	120.10	110.20
2	O	312	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	R	434	ASP	CA-CB-CG	-5.20	101.95	113.40
1	A	38	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	62	LEU	CA-CB-CG	5.19	127.23	115.30
2	R	367	PHE	CA-C-O	-5.19	109.21	120.10
1	F	133	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	R	440	ARG	CD-NE-CZ	5.17	130.84	123.60
1	E	174	ARG	CD-NE-CZ	-5.17	116.36	123.60
1	D	177	VAL	CB-CA-C	5.17	121.21	111.40
2	R	313	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	M	376	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	F	106	LEU	N-CA-CB	-5.15	100.09	110.40
2	M	313	ARG	CD-NE-CZ	5.15	130.81	123.60
2	R	434	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	176	GLU	CG-CD-OE1	5.14	128.58	118.30
2	O	474	LEU	N-CA-CB	-5.14	100.12	110.40
1	F	178	ASP	CB-CG-OD1	5.14	122.92	118.30
2	P	372	LEU	N-CA-CB	-5.13	100.14	110.40
1	A	94	ARG	CG-CD-NE	5.13	122.57	111.80
1	C	85	LEU	CB-CA-C	5.12	119.94	110.20
2	P	383	ARG	NH1-CZ-NH2	5.12	125.03	119.40
2	R	521	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	A	3	GLU	CA-CB-CG	5.11	124.63	113.40
2	O	372	LEU	CA-CB-CG	5.09	127.02	115.30
1	F	99	PHE	CB-CA-C	5.09	120.58	110.40
1	D	176	GLU	CG-CD-OE1	5.09	128.47	118.30
2	R	440	ARG	CB-CG-CD	-5.09	98.37	111.60
2	R	383	ARG	CD-NE-CZ	-5.08	116.48	123.60
2	Q	440	ARG	CB-CG-CD	-5.08	98.39	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	GLN	N-CA-CB	-5.07	101.47	110.60
2	N	362	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	36	TRP	CB-CA-C	5.06	120.52	110.40
2	R	434	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	C	106	LEU	CB-CG-CD2	-5.06	102.40	111.00
2	N	314	ASN	N-CA-CB	5.05	119.70	110.60
2	O	524	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	186	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	176	GLU	CB-CG-CD	5.04	127.81	114.20
1	B	142	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	P	409	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	P	519	LEU	CB-CA-C	5.03	119.76	110.20
2	N	451	ASN	CB-CG-OD1	-5.03	111.55	121.60
1	D	40	ALA	CB-CA-C	-5.03	102.56	110.10
1	E	38	ARG	CD-NE-CZ	-5.02	116.57	123.60
1	D	94	ARG	CB-CG-CD	5.02	124.65	111.60
2	Q	452	GLY	N-CA-C	-5.02	100.56	113.10
2	N	367	PHE	CA-C-O	-5.01	109.57	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	34	0
1	B	1571	0	1499	45	0
1	C	1571	0	1499	43	0
1	D	1571	0	1499	29	0
1	E	1571	0	1499	42	0
1	F	1571	0	1499	49	0
2	M	1840	0	1793	51	0
2	N	1840	0	1793	32	0
2	O	1840	0	1793	34	0
2	P	1840	0	1793	48	0
2	Q	1840	0	1793	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1840	0	1793	63	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	A	83	0	0	2	0
4	B	79	0	0	1	0
4	C	80	0	0	2	0
4	D	77	0	0	0	0
4	E	77	0	0	0	0
4	F	83	0	0	1	0
4	M	154	0	0	4	0
4	N	163	0	0	2	0
4	O	158	0	0	5	0
4	P	159	0	0	1	0
4	Q	163	0	0	6	0
4	R	158	0	0	4	0
All	All	21906	0	19752	475	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 12.

All (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:NE2	1:E:165:GLN:H	1.34	1.23
1:E:165:GLN:N	1:E:165:GLN:HE21	1.39	1.18
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.68	1.07
1:B:165:GLN:NE2	1:B:165:GLN:H	1.64	0.95
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.68	0.94
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.48	0.93
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.51	0.92
1:B:176:GLU:HG3	1:B:180:LYS:O	1.68	0.92
2:R:411:LYS:O	2:R:414:ARG:NH1	2.04	0.90
2:Q:411:LYS:H	2:Q:411:LYS:HE2	1.38	0.88
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.39	0.86
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.91	0.86
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.38	0.86
2:Q:411:LYS:H	2:Q:411:LYS:CE	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:522:ARG:NH1	4:O:673:HOH:O	2.12	0.82
1:C:44:ALA:O	1:C:48:HIS:NE2	2.13	0.81
2:R:361:HIS:H	2:R:361:HIS:CD2	1.98	0.81
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.45	0.80
1:F:177:VAL:O	1:F:180:LYS:HB3	1.82	0.79
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.18	0.79
2:R:497:ASN:ND2	2:R:499:GLU:H	1.80	0.78
2:N:522:ARG:NH1	4:N:673:HOH:O	2.17	0.78
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.48	0.78
2:O:497:ASN:HD22	2:O:499:GLU:H	1.30	0.77
2:M:522:ARG:NH1	4:M:661:HOH:O	2.17	0.77
2:Q:411:LYS:N	2:Q:411:LYS:HE2	1.99	0.77
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.99	0.77
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.65	0.77
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.48	0.76
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.19	0.76
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.16	0.75
2:M:497:ASN:ND2	2:M:499:GLU:H	1.84	0.75
2:M:361:HIS:H	2:M:361:HIS:CD2	2.06	0.73
1:C:26:ALA:O	2:O:411:LYS:NZ	2.16	0.73
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.68	0.73
1:B:65:ASP:OD2	1:B:133:ARG:HD3	1.89	0.73
2:N:411:LYS:H	2:N:411:LYS:CE	2.02	0.73
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.04	0.73
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.23	0.72
2:R:411:LYS:CE	2:R:411:LYS:H	2.02	0.72
1:B:165:GLN:HE21	1:B:165:GLN:H	1.39	0.71
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.25	0.71
2:P:411:LYS:H	2:P:411:LYS:CE	2.04	0.71
1:D:180:LYS:HG3	1:D:181:THR:N	2.06	0.71
2:P:497:ASN:HD22	2:P:499:GLU:H	1.39	0.71
2:O:497:ASN:ND2	2:O:499:GLU:H	1.89	0.70
1:A:176:GLU:HG3	1:A:180:LYS:O	1.91	0.70
2:Q:522:ARG:NH1	4:Q:1072:HOH:O	2.24	0.70
2:N:411:LYS:HE2	2:N:411:LYS:H	1.56	0.70
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.74	0.70
2:R:361:HIS:H	2:R:361:HIS:HD2	1.40	0.69
1:B:176:GLU:HG3	1:B:180:LYS:C	2.14	0.68
1:D:1:PRO:HG2	2:R:488:MET:HE1	1.75	0.68
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.92	0.68
1:F:165:GLN:NE2	1:F:165:GLN:H	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.57	0.67
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.41	0.67
2:R:497:ASN:HD22	2:R:497:ASN:C	1.98	0.67
1:D:176:GLU:HA	1:D:180:LYS:O	1.95	0.67
2:N:361:HIS:H	2:N:361:HIS:CD2	2.12	0.66
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.59	0.66
2:N:497:ASN:HD22	2:N:499:GLU:H	1.42	0.66
2:M:376:GLU:OE1	4:M:632:HOH:O	2.14	0.66
2:P:411:LYS:O	2:P:414:ARG:NH1	2.29	0.66
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.96	0.66
1:F:23:LEU:O	1:F:26:ALA:HB3	1.96	0.66
2:O:411:LYS:CE	2:O:411:LYS:H	2.08	0.66
1:E:24:GLU:O	1:E:27:GLY:N	2.29	0.66
2:Q:306:SER:OG	2:Q:530:GLN:NE2	2.22	0.66
2:P:361:HIS:CD2	2:P:361:HIS:H	2.15	0.65
2:R:411:LYS:H	2:R:411:LYS:HE2	1.61	0.65
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.10	0.65
1:C:35:ILE:HG22	1:C:94:ARG:HD3	1.78	0.65
2:M:361:HIS:HD2	2:M:361:HIS:H	1.45	0.65
2:M:390:LYS:HD2	4:M:637:HOH:O	1.97	0.65
2:R:497:ASN:HD22	2:R:498:PRO:N	1.95	0.64
1:B:26:ALA:O	2:N:411:LYS:NZ	2.23	0.64
2:M:497:ASN:HD22	2:M:499:GLU:H	1.44	0.64
2:P:414:ARG:HA	2:P:414:ARG:NE	2.13	0.64
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.12	0.64
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.18	0.64
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.80	0.64
2:P:497:ASN:ND2	2:P:499:GLU:H	1.95	0.64
1:A:65:ASP:OD2	1:A:133:ARG:HD3	1.99	0.63
2:O:361:HIS:CD2	2:O:361:HIS:H	2.17	0.63
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.13	0.63
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.19	0.63
1:D:165:GLN:H	1:D:165:GLN:HE21	1.46	0.63
1:F:176:GLU:HG3	1:F:180:LYS:H	1.64	0.62
1:B:39:LEU:HD13	1:B:106:LEU:HD21	1.81	0.62
2:R:497:ASN:HD22	2:R:499:GLU:H	1.42	0.62
1:A:176:GLU:HA	1:A:180:LYS:O	1.99	0.62
1:C:52:LEU:HD23	1:C:103:GLU:CD	2.20	0.62
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.32	0.62
2:R:390:LYS:HE2	4:R:1433:HOH:O	1.99	0.62
1:C:103:GLU:OE2	1:C:184:ARG:NH1	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.81	0.61
1:C:35:ILE:CG2	1:C:94:ARG:HD3	2.29	0.61
2:Q:411:LYS:O	2:Q:414:ARG:NH1	2.32	0.61
2:M:413:ASP:O	2:M:414:ARG:NH1	2.33	0.61
1:E:26:ALA:O	2:Q:411:LYS:NZ	2.28	0.61
1:D:35:ILE:HG22	1:D:94:ARG:HG3	1.83	0.61
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.64	0.60
2:O:376:GLU:O	2:O:442:ILE:HA	2.01	0.60
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.36	0.60
1:C:165:GLN:H	1:C:165:GLN:NE2	1.99	0.59
1:D:165:GLN:H	1:D:165:GLN:NE2	1.99	0.59
1:F:80:GLN:O	1:F:91:SER:HB2	2.01	0.59
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.67	0.59
2:O:411:LYS:H	2:O:411:LYS:HE2	1.66	0.59
2:M:411:LYS:O	2:M:414:ARG:NH1	2.35	0.59
2:R:318:LYS:HE2	4:R:1430:HOH:O	2.02	0.59
1:F:133:ARG:HG3	2:R:326:THR:HG21	1.84	0.59
2:P:376:GLU:O	2:P:442:ILE:HA	2.03	0.59
2:P:411:LYS:HE2	2:P:411:LYS:H	1.68	0.58
2:P:315:TRP:HZ2	2:P:503:GLN:NE2	2.01	0.58
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.39	0.58
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.68	0.58
1:F:147:ASP:OD2	1:F:174:ARG:CD	2.51	0.58
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.52	0.58
2:N:411:LYS:HE2	2:N:411:LYS:N	2.18	0.58
1:F:176:GLU:HG3	1:F:180:LYS:N	2.19	0.57
2:P:522:ARG:NH1	4:P:674:HOH:O	2.34	0.57
1:F:26:ALA:O	2:R:411:LYS:NZ	2.29	0.57
2:M:304:ASP:HB2	2:M:343:ILE:HG13	1.85	0.57
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.05	0.57
1:A:163:GLN:HB2	4:A:278:HOH:O	2.04	0.57
1:F:24:GLU:O	1:F:27:GLY:N	2.37	0.57
2:N:497:ASN:ND2	2:N:499:GLU:H	2.03	0.57
1:C:41:LYS:O	1:C:44:ALA:N	2.38	0.57
2:O:413:ASP:C	2:O:414:ARG:HD2	2.25	0.57
1:C:64:ARG:O	1:C:98:THR:HA	2.05	0.56
1:F:50:LEU:HD12	1:F:51:LEU:N	2.21	0.56
2:P:414:ARG:HA	2:P:414:ARG:HE	1.69	0.56
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.87	0.56
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.87	0.56
2:R:522:ARG:NH1	4:R:1311:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LYS:O	1:C:43:ASP:N	2.39	0.56
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.88	0.56
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.04	0.56
2:N:414:ARG:HA	2:N:414:ARG:NE	2.21	0.56
2:M:411:LYS:HD3	2:M:411:LYS:H	1.71	0.56
1:F:174:ARG:HD2	1:F:183:TYR:CE2	2.41	0.55
2:M:497:ASN:HD22	2:M:498:PRO:N	2.05	0.55
1:B:176:GLU:HA	1:B:180:LYS:O	2.07	0.55
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.05	0.55
1:E:188:ARG:NH1	1:E:188:ARG:HG3	2.21	0.54
1:E:54:GLN:OE1	1:E:184:ARG:NH2	2.40	0.54
2:O:390:LYS:HE2	4:O:730:HOH:O	2.08	0.54
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.42	0.54
2:Q:411:LYS:H	2:Q:411:LYS:CD	2.19	0.54
2:R:399:MET:HA	2:R:462:HIS:O	2.07	0.54
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.36	0.54
1:B:176:GLU:OE2	1:B:179:GLY:C	2.46	0.54
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.43	0.54
2:N:361:HIS:HD2	2:N:361:HIS:H	1.52	0.54
2:P:325:LYS:HD3	2:Q:335:ALA:HB1	1.89	0.54
2:R:361:HIS:N	2:R:361:HIS:CD2	2.68	0.54
1:A:165:GLN:H	1:A:165:GLN:CD	2.11	0.54
1:A:155:CYS:O	1:A:159:ASN:ND2	2.35	0.54
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.22	0.54
2:Q:414:ARG:N	2:Q:414:ARG:HD2	2.22	0.53
1:E:133:ARG:HG3	2:Q:326:THR:HG21	1.91	0.53
2:M:414:ARG:HD2	2:M:414:ARG:N	2.23	0.53
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.44	0.53
2:M:411:LYS:H	2:M:411:LYS:CD	2.21	0.53
2:N:359:HIS:O	2:N:366:ASN:HB3	2.07	0.53
1:F:163:GLN:HB3	1:F:165:GLN:HE21	1.70	0.53
1:F:47:GLU:O	1:F:49:ILE:HG23	2.09	0.53
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.12	0.53
1:B:165:GLN:N	1:B:165:GLN:HE21	2.05	0.53
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.09	0.53
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.91	0.52
2:O:362:ASP:OD1	2:O:440:ARG:HD3	2.08	0.52
1:C:143:LEU:HD23	1:C:143:LEU:C	2.30	0.52
1:A:84:ASN:OD1	1:A:86:GLU:HB2	2.10	0.52
2:P:313:ARG:O	2:P:318:LYS:HE3	2.09	0.52
1:E:94:ARG:NH2	2:Q:398:GLU:OE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.27	0.52
1:B:176:GLU:HG3	1:B:180:LYS:N	2.24	0.52
1:C:114:VAL:HG22	4:C:234:HOH:O	2.08	0.52
2:N:414:ARG:CA	2:N:414:ARG:NE	2.72	0.52
1:B:19:ILE:O	2:N:426:VAL:HG21	2.09	0.52
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.31	0.52
1:E:20:GLY:O	1:E:21:LEU:HD23	2.10	0.52
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.91	0.52
1:A:36:TRP:HA	1:A:36:TRP:CE3	2.45	0.52
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.46	0.51
1:B:176:GLU:CG	1:B:180:LYS:N	2.73	0.51
1:C:108:THR:OG1	1:C:109:VAL:N	2.43	0.51
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.91	0.51
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.76	0.51
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.73	0.51
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.93	0.51
2:R:376:GLU:O	2:R:442:ILE:HA	2.10	0.51
1:A:64:ARG:O	1:A:98:THR:HA	2.10	0.51
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.25	0.51
2:M:376:GLU:O	2:M:442:ILE:HA	2.11	0.51
2:P:361:HIS:HD2	2:P:361:HIS:H	1.55	0.51
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.92	0.50
1:F:176:GLU:HA	1:F:180:LYS:O	2.11	0.50
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.93	0.50
1:A:143:LEU:HD23	1:A:143:LEU:C	2.31	0.50
1:D:26:ALA:O	2:P:411:LYS:NZ	2.41	0.50
1:C:163:GLN:CB	1:C:165:GLN:NE2	2.59	0.50
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.93	0.50
1:C:177:VAL:O	1:C:180:LYS:HB3	2.11	0.50
1:F:74:ASP:HB2	4:F:1285:HOH:O	2.11	0.50
2:Q:410:HIS:ND1	2:Q:411:LYS:HE2	2.27	0.50
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.47	0.50
1:B:165:GLN:N	1:B:165:GLN:NE2	2.46	0.49
1:C:131:PHE:O	1:C:132:ALA:HB2	2.12	0.49
1:F:53:GLY:HA3	1:F:185:PHE:O	2.11	0.49
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.93	0.49
2:R:359:HIS:O	2:R:366:ASN:HB3	2.13	0.49
1:C:63:VAL:HG12	1:C:66:SER:HB3	1.93	0.49
2:R:410:HIS:ND1	2:R:411:LYS:HE2	2.27	0.49
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.12	0.49
1:B:170:LEU:HD21	1:B:196:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:497:ASN:ND2	2:P:499:GLU:OE1	2.42	0.49
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.41	0.49
1:B:23:LEU:N	1:B:23:LEU:HD12	2.28	0.49
2:M:386:ASP:HA	2:M:527:LEU:O	2.13	0.49
2:O:326:THR:HG22	2:O:326:THR:O	2.13	0.49
1:C:89:PHE:CE1	1:C:109:VAL:HG22	2.47	0.48
2:P:399:MET:HA	2:P:462:HIS:O	2.13	0.48
1:E:176:GLU:HA	1:E:180:LYS:O	2.13	0.48
1:B:74:ASP:OD2	1:B:80:GLN:NE2	2.45	0.48
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.29	0.48
1:B:94:ARG:NH2	2:N:398:GLU:OE2	2.45	0.48
2:O:307:ARG:HG2	2:O:533:THR:HG22	1.96	0.48
2:Q:497:ASN:ND2	2:Q:499:GLU:HB2	2.28	0.48
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.28	0.48
1:B:163:GLN:HA	1:B:164:PRO:HD2	1.67	0.48
1:B:74:ASP:HB2	4:B:329:HOH:O	2.12	0.48
2:N:360:ASP:OD2	2:N:428:ARG:HD2	2.13	0.48
2:M:497:ASN:HD22	2:M:497:ASN:C	2.16	0.48
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.10	0.48
2:R:411:LYS:CD	2:R:411:LYS:H	2.27	0.48
1:A:176:GLU:OE2	1:A:179:GLY:HA2	2.14	0.48
1:B:51:LEU:O	1:B:105:THR:HA	2.13	0.48
1:C:47:GLU:O	1:C:49:ILE:HG23	2.12	0.48
2:N:376:GLU:O	2:N:442:ILE:HA	2.14	0.48
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.61	0.48
2:R:306:SER:OG	2:R:530:GLN:NE2	2.39	0.48
1:E:44:ALA:O	1:E:48:HIS:NE2	2.32	0.48
1:F:36:TRP:CD1	1:F:37:ASN:OD1	2.67	0.48
2:P:411:LYS:H	2:P:411:LYS:NZ	2.12	0.48
2:R:363:LEU:HD23	2:R:425:GLY:HA2	1.96	0.48
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.96	0.48
1:B:84:ASN:OD1	1:B:86:GLU:HB2	2.14	0.47
2:P:497:ASN:C	2:P:497:ASN:HD22	2.18	0.47
2:Q:376:GLU:OE1	4:Q:1021:HOH:O	2.20	0.47
2:N:333:ARG:HH11	2:N:333:ARG:HD3	1.44	0.47
2:N:399:MET:HA	2:N:462:HIS:O	2.14	0.47
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.80	0.47
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.95	0.47
2:P:356:PHE:HD1	2:P:428:ARG:HD3	1.80	0.47
1:E:6:PRO:HG2	2:Q:503:GLN:NE2	2.29	0.47
2:R:306:SER:CB	2:R:530:GLN:HE21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:O	1:D:180:LYS:HB3	2.14	0.47
2:Q:390:LYS:HE2	4:Q:1154:HOH:O	2.13	0.47
1:F:19:ILE:O	2:R:426:VAL:HG21	2.14	0.47
2:R:354:LEU:HD21	2:R:428:ARG:NH2	2.29	0.47
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.50	0.47
1:C:120:VAL:CG1	1:C:156:PRO:HG3	2.45	0.47
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.95	0.47
2:R:411:LYS:N	2:R:411:LYS:HE2	2.29	0.47
2:N:411:LYS:CD	2:N:411:LYS:H	2.28	0.47
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.13	0.47
2:O:361:HIS:HD2	2:O:361:HIS:H	1.63	0.47
1:A:50:LEU:O	1:A:182:ALA:HA	2.15	0.47
1:B:39:LEU:HD13	1:B:106:LEU:CD2	2.44	0.47
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.50	0.47
1:A:78:GLU:OE1	2:M:301:PRO:HG3	2.15	0.47
2:O:381:ALA:O	2:O:522:ARG:HA	2.14	0.47
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.97	0.47
1:A:51:LEU:HD11	1:A:126:ILE:HD12	1.97	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.15	0.47
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.76	0.46
2:R:364:LEU:HB2	2:R:440:ARG:HD3	1.96	0.46
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.45	0.46
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.97	0.46
2:Q:454:ASN:HB2	2:R:310:ILE:HG13	1.96	0.46
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.53	0.46
1:F:165:GLN:CD	1:F:165:GLN:H	2.18	0.46
2:M:410:HIS:ND1	2:M:411:LYS:HE2	2.30	0.46
2:Q:364:LEU:HD13	2:Q:441:THR:HA	1.97	0.46
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.15	0.46
1:D:143:LEU:HD23	1:D:143:LEU:C	2.36	0.46
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.85	0.46
2:O:473:LYS:NZ	4:O:721:HOH:O	2.32	0.46
2:P:310:ILE:HD12	2:R:453:PRO:HB2	1.96	0.46
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.84	0.46
1:D:26:ALA:O	2:P:411:LYS:HE3	2.16	0.46
2:O:414:ARG:N	2:O:414:ARG:HD2	2.31	0.46
2:Q:390:LYS:HD2	4:Q:1033:HOH:O	2.16	0.46
1:E:8:THR:HA	1:E:9:PRO:HD3	1.80	0.46
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.16	0.46
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.46	0.46
1:F:178:ASP:O	1:F:179:GLY:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:GLN:NE2	2:R:355:GLY:HA3	2.31	0.46
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.71	0.46
1:D:177:VAL:O	1:D:180:LYS:N	2.47	0.46
2:N:478:LEU:C	2:N:478:LEU:HD23	2.36	0.46
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.27	0.46
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.98	0.46
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.16	0.46
2:R:413:ASP:C	2:R:414:ARG:HD2	2.36	0.46
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.46	0.46
1:F:131:PHE:O	1:F:132:ALA:HB2	2.16	0.45
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.15	0.45
1:F:41:LYS:HE3	1:F:85:LEU:O	2.15	0.45
2:R:386:ASP:HA	2:R:527:LEU:O	2.16	0.45
2:R:522:ARG:NH2	2:R:524:ASP:OD1	2.46	0.45
2:O:403:ASN:HB2	4:O:613:HOH:O	2.16	0.45
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.47	0.45
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.17	0.45
1:D:72:GLN:O	1:D:91:SER:OG	2.31	0.45
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.97	0.45
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.16	0.45
1:B:143:LEU:HD23	1:B:143:LEU:C	2.36	0.45
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.46	0.45
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.85	0.45
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.51	0.45
2:R:447:TYR:HB2	2:R:448:PRO:HD2	1.97	0.45
1:E:41:LYS:HD2	1:E:87:ASN:O	2.17	0.45
1:E:47:GLU:O	1:E:49:ILE:HG23	2.17	0.45
2:M:410:HIS:CE1	2:M:411:LYS:CE	3.00	0.45
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.50	0.45
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.65	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.37	0.45
2:O:400:TRP:HA	2:O:425:GLY:O	2.17	0.45
1:E:31:ARG:HH12	2:Q:428:ARG:HG2	1.80	0.45
2:R:414:ARG:N	2:R:414:ARG:HD2	2.32	0.45
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.99	0.45
2:M:405:GLY:HA3	4:M:641:HOH:O	2.16	0.45
2:M:413:ASP:C	2:M:414:ARG:HD2	2.37	0.45
1:D:26:ALA:O	2:P:411:LYS:CE	2.65	0.45
1:D:51:LEU:HD11	1:D:126:ILE:HD12	1.99	0.45
2:Q:536:GLU:HB2	4:Q:1116:HOH:O	2.15	0.45
1:D:33:GLN:HG2	1:D:85:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:ASN:OD1	1:E:116:ASN:C	2.53	0.44
2:O:478:LEU:C	2:O:478:LEU:HD23	2.37	0.44
1:B:146:ASP:HB3	1:B:171:ILE:HG22	1.99	0.44
1:F:52:LEU:O	1:F:184:ARG:HA	2.16	0.44
2:Q:460:HIS:HA	2:Q:478:LEU:O	2.18	0.44
2:M:302:ALA:HB1	2:M:347:THR:CG2	2.48	0.44
1:C:4:LEU:HB3	2:O:387:GLN:HB3	1.99	0.44
1:E:164:PRO:N	1:E:165:GLN:NE2	2.65	0.44
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.48	0.44
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.99	0.44
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.66	0.44
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.73	0.44
1:D:19:ILE:O	2:P:426:VAL:HG21	2.18	0.44
1:B:62:LEU:HD12	1:B:64:ARG:NH2	2.33	0.44
1:F:160:LEU:HD23	1:F:160:LEU:HA	1.88	0.44
2:M:410:HIS:CE1	2:M:411:LYS:HZ1	2.35	0.44
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.81	0.44
1:D:61:HIS:CD2	1:E:165:GLN:OE1	2.70	0.44
1:F:115:ASN:HA	1:F:121:PRO:HA	2.00	0.44
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.78	0.44
2:R:392:VAL:HG12	2:R:395:THR:HB	1.99	0.44
2:R:408:TYR:HE2	2:R:447:TYR:CZ	2.36	0.44
1:C:50:LEU:O	1:C:182:ALA:HA	2.17	0.44
1:E:41:LYS:O	1:E:44:ALA:N	2.45	0.44
1:A:35:ILE:HG22	1:A:94:ARG:HG3	2.00	0.43
1:D:146:ASP:HB3	1:D:171:ILE:HG22	2.00	0.43
2:P:359:HIS:O	2:P:366:ASN:HB3	2.17	0.43
1:B:165:GLN:CD	1:B:165:GLN:H	2.19	0.43
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.48	0.43
2:Q:429:CYS:SG	4:Q:1122:HOH:O	2.12	0.43
2:R:385:VAL:O	2:R:526:VAL:HA	2.19	0.43
1:A:163:GLN:HG3	1:C:61:HIS:CE1	2.54	0.43
1:C:163:GLN:CB	1:C:165:GLN:HE22	2.27	0.43
1:F:51:LEU:HD11	1:F:126:ILE:CD1	2.48	0.43
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.39	0.43
2:P:484:PRO:O	2:P:488:MET:HE2	2.18	0.43
2:R:383:ARG:HA	2:R:435:GLY:O	2.18	0.43
1:D:1:PRO:HG2	2:R:488:MET:CE	2.47	0.43
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.65	0.43
2:P:486:ILE:HB	2:P:487:PRO:HD3	2.00	0.43
2:M:305:ASN:O	2:M:533:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:410:HIS:CE1	2:M:411:LYS:HE2	2.54	0.43
2:R:410:HIS:CE1	2:R:411:LYS:HE2	2.54	0.43
1:E:39:LEU:HD11	1:E:93:GLY:HA3	2.01	0.43
2:P:489:CYS:O	2:P:493:LYS:HG3	2.19	0.43
2:P:315:TRP:CZ2	2:P:503:GLN:NE2	2.86	0.43
1:B:40:ALA:HB2	1:B:89:PHE:HD1	1.81	0.42
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.91	0.42
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.18	0.42
1:C:24:GLU:O	1:C:27:GLY:N	2.46	0.42
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.73	0.42
1:A:180:LYS:CG	1:A:181:THR:N	2.82	0.42
2:M:335:ALA:HB2	2:O:328:ILE:HD12	2.01	0.42
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.38	0.42
2:R:497:ASN:ND2	2:R:497:ASN:C	2.68	0.42
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.79	0.42
1:C:52:LEU:HA	1:C:104:TRP:O	2.19	0.42
1:C:41:LYS:O	1:C:42:PRO:C	2.58	0.42
1:E:165:GLN:H	1:E:165:GLN:HE21	0.58	0.42
1:E:165:GLN:NE2	1:E:165:GLN:N	2.20	0.42
1:F:157:VAL:O	1:F:160:LEU:HB2	2.19	0.42
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.84	0.42
1:E:176:GLU:HG2	1:E:179:GLY:HA2	2.01	0.42
2:M:410:HIS:CE1	2:M:411:LYS:NZ	2.88	0.42
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.38	0.42
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.02	0.42
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.35	0.42
1:A:28:ASN:HB3	4:A:271:HOH:O	2.20	0.42
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.51	0.42
2:M:446:PRO:HD2	2:P:376:GLU:HG2	2.00	0.42
2:P:497:ASN:HD22	2:P:499:GLU:N	2.14	0.42
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.80	0.42
2:R:400:TRP:HA	2:R:425:GLY:O	2.19	0.42
2:P:497:ASN:HD22	2:P:498:PRO:N	2.17	0.42
1:B:8:THR:HA	1:B:9:PRO:HD3	1.86	0.41
2:M:399:MET:HA	2:M:462:HIS:O	2.20	0.41
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.86	0.41
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.50	0.41
1:E:143:LEU:HD12	1:E:185:PHE:CG	2.55	0.41
2:N:415:TYR:CE1	2:N:416:LEU:HD23	2.56	0.41
1:C:161:ILE:HD13	1:C:196:VAL:HG21	2.02	0.41
1:C:64:ARG:HG2	1:C:64:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:416:LEU:HD23	2:M:416:LEU:C	2.39	0.41
2:N:411:LYS:HE2	2:N:411:LYS:HB2	1.74	0.41
1:C:51:LEU:O	1:C:105:THR:HA	2.20	0.41
2:M:478:LEU:C	2:M:478:LEU:HD23	2.41	0.41
2:N:450:ARG:HG3	4:N:639:HOH:O	2.20	0.41
2:P:411:LYS:HE2	2:P:411:LYS:N	2.35	0.41
2:R:363:LEU:HD12	2:R:363:LEU:N	2.35	0.41
2:R:473:LYS:NZ	4:R:1378:HOH:O	2.28	0.41
1:D:1:PRO:CG	2:R:488:MET:HE1	2.48	0.41
1:B:39:LEU:HD11	1:B:93:GLY:HA3	2.02	0.41
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.36	0.41
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.21	0.41
1:B:190:GLN:HG3	2:N:333:ARG:HG2	2.01	0.41
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.36	0.41
2:M:448:PRO:HB2	2:P:516:MET:HA	2.02	0.41
1:C:41:LYS:C	1:C:43:ASP:N	2.73	0.41
2:M:302:ALA:HB1	2:M:347:THR:HG21	2.02	0.41
2:O:359:HIS:O	2:O:366:ASN:HB3	2.21	0.41
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.84	0.41
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.56	0.41
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.82	0.41
1:B:163:GLN:O	1:B:166:ARG:N	2.52	0.41
2:M:363:LEU:HD11	2:M:427:GLY:HA3	2.03	0.41
2:P:478:LEU:HD23	2:P:478:LEU:C	2.41	0.41
1:D:5:LEU:O	2:P:387:GLN:HG2	2.21	0.41
2:M:379:ILE:HD13	2:Q:534:HIS:CE1	2.56	0.41
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.56	0.40
1:C:28:ASN:HB3	4:C:270:HOH:O	2.21	0.40
1:E:52:LEU:HD23	1:E:103:GLU:OE1	2.21	0.40
1:F:120:VAL:HA	1:F:121:PRO:HD2	1.93	0.40
2:O:443:LYS:HE3	2:O:480:PHE:CG	2.56	0.40
2:P:350:ASN:OD1	2:P:350:ASN:C	2.59	0.40
2:O:390:LYS:CE	4:O:730:HOH:O	2.65	0.40
2:O:497:ASN:HD22	2:O:497:ASN:C	2.24	0.40
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.67	0.40
2:P:484:PRO:O	2:P:488:MET:CE	2.69	0.40
2:R:437:TYR:C	2:R:437:TYR:CD1	2.95	0.40
2:R:378:ILE:HA	2:R:519:LEU:O	2.21	0.40
1:A:131:PHE:O	1:A:132:ALA:HB2	2.21	0.40
1:A:188:ARG:HH11	1:A:188:ARG:HG3	1.87	0.40
1:B:52:LEU:HA	1:B:104:TRP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.97	0.40
1:F:36:TRP:CG	1:F:37:ASN:N	2.89	0.40
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.37	0.40
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.56	0.40
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.70	0.40
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.85	0.40
1:C:35:ILE:HG22	1:C:94:ARG:CD	2.49	0.40
1:F:50:LEU:O	1:F:182:ALA:HA	2.21	0.40
2:P:410:HIS:HA	2:P:411:LYS:HZ1	1.87	0.40
2:R:364:LEU:HD11	2:R:442:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
1	C	198/200 (99%)	193 (98%)	4 (2%)	1 (0%)	29	22
1	D	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	185 (93%)	13 (7%)	0	100	100
2	M	229/238 (96%)	224 (98%)	5 (2%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	224 (98%)	5 (2%)	0	100	100
2	Q	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	R	229/238 (96%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2562/2628 (98%)	2472 (96%)	89 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	151 (93%)	11 (7%)	16	10
1	B	162/163 (99%)	155 (96%)	7 (4%)	29	27
1	C	162/163 (99%)	157 (97%)	5 (3%)	40	39
1	D	162/163 (99%)	152 (94%)	10 (6%)	18	14
1	E	162/163 (99%)	158 (98%)	4 (2%)	47	49
1	F	162/163 (99%)	155 (96%)	7 (4%)	29	27
2	M	196/202 (97%)	187 (95%)	9 (5%)	27	23
2	N	196/202 (97%)	186 (95%)	10 (5%)	24	20
2	O	196/202 (97%)	185 (94%)	11 (6%)	21	16
2	P	196/202 (97%)	185 (94%)	11 (6%)	21	16
2	Q	196/202 (97%)	186 (95%)	10 (5%)	24	20
2	R	196/202 (97%)	187 (95%)	9 (5%)	27	23
All	All	2148/2190 (98%)	2044 (95%)	104 (5%)	25	22

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG

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Mol	Chain	Res	Type
1	A	43	ASP
1	A	52	LEU
1	A	94	ARG
1	A	106	LEU
1	A	133	ARG
1	A	143	LEU
1	A	165	GLN
1	A	192	GLU
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	428	ARG
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	52	LEU
1	B	106	LEU
1	B	154	LYS
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	411	LYS
2	N	416	LEU
2	N	478	LEU
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	38	ARG
1	C	52	LEU
1	C	133	ARG
1	C	165	GLN
2	O	372	LEU
2	O	393	PRO
2	O	395	THR

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Mol	Chain	Res	Type
2	O	411	LYS
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	442	ILE
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	42	PRO
1	D	52	LEU
1	D	91	SER
1	D	133	ARG
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	395	THR
2	P	411	LYS
2	P	414	ARG
2	P	416	LEU
2	P	434	ASP
2	P	438	SER
2	P	440	ARG
2	P	478	LEU
2	P	497	ASN
2	P	511	ASN
2	P	534	HIS
1	E	4	LEU
1	E	52	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	395	THR
2	Q	399	MET
2	Q	411	LYS
2	Q	416	LEU
2	Q	428	ARG
2	Q	442	ILE
2	Q	497	ASN
2	Q	499	GLU
2	Q	507	LYS

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Mol	Chain	Res	Type
2	Q	534	HIS
1	F	4	LEU
1	F	30	THR
1	F	52	LEU
1	F	91	SER
1	F	133	ARG
1	F	165	GLN
1	F	181	THR
2	R	372	LEU
2	R	395	THR
2	R	411	LYS
2	R	416	LEU
2	R	428	ARG
2	R	473	LYS
2	R	497	ASN
2	R	507	LYS
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

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

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Mol	Chain	Res	Type
2	P	503	GLN
1	E	107	HIS
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.