Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:37 AM GMT

PDB ID	:	3PCN
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3,4-DIHYDROXYPHENYLACETATE
Authors	:	Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-08-19
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/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:

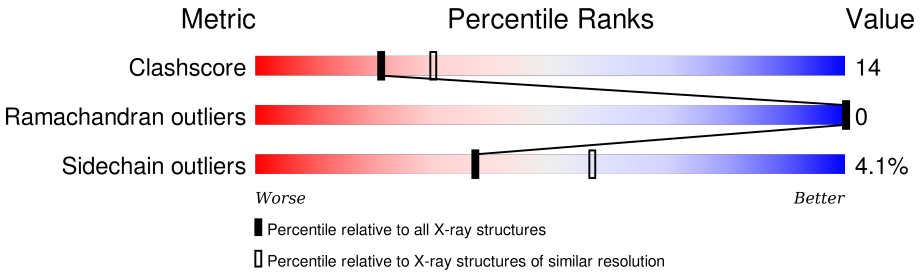
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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. 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 <=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	74% 22%
1	B	200	73% 23%
1	C	200	74% 24%
1	D	200	71% 25%
1	E	200	71% 26%
1	F	200	72% 25%
2	M	238	71% 23%

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Mol	Chain	Length	Quality of chain
2	N	238	73% 23%
2	O	238	73% 23%
2	P	238	72% 23%
2	Q	238	67% 26% 5%
2	R	238	66% 29%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DHY	Q	550[A]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

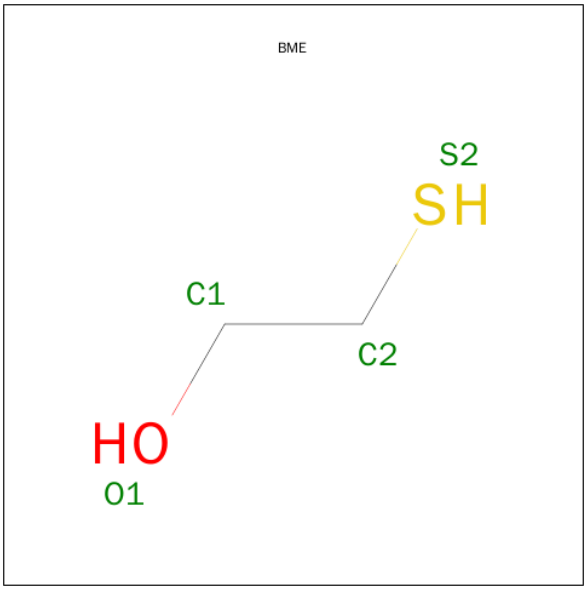
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

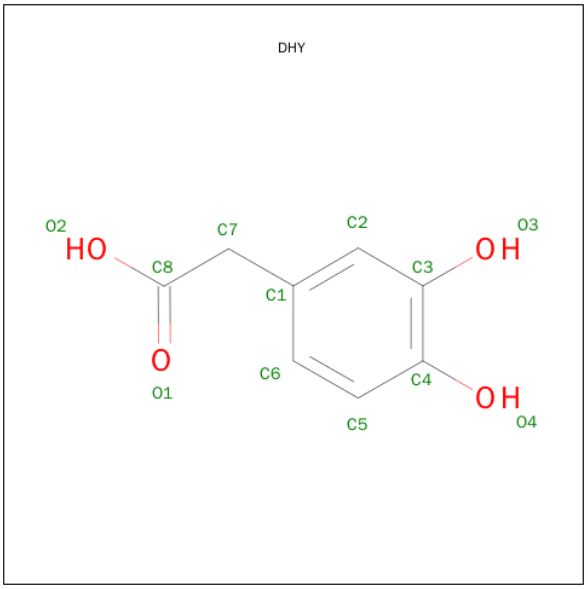
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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

- Molecule 5 is 2-(3,4-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: DHY) (formula: $C_8H_8O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 24 16 8	0	1
5	N	1	Total C O 24 16 8	0	1
5	O	1	Total C O 24 16 8	0	1
5	P	1	Total C O 24 16 8	0	1
5	Q	1	Total C O 24 16 8	0	1
5	R	1	Total C O 24 16 8	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	80	Total O 80 80	0	0
6	B	79	Total O 79 79	0	0
6	C	81	Total O 81 81	0	0
6	D	82	Total O 82 82	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	80	Total O 80 80	0	0
6	F	79	Total O 79 79	0	0
6	M	150	Total O 150 150	0	0
6	N	152	Total O 152 152	0	0
6	O	147	Total O 147 147	0	0
6	P	145	Total O 145 145	0	0
6	Q	149	Total O 149 149	0	0
6	R	150	Total O 150 150	0	0

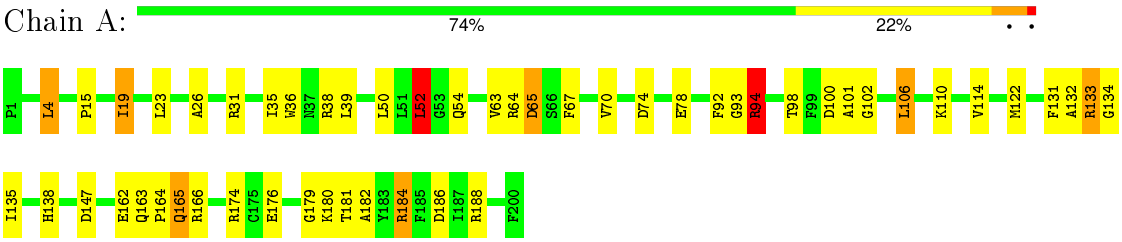
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

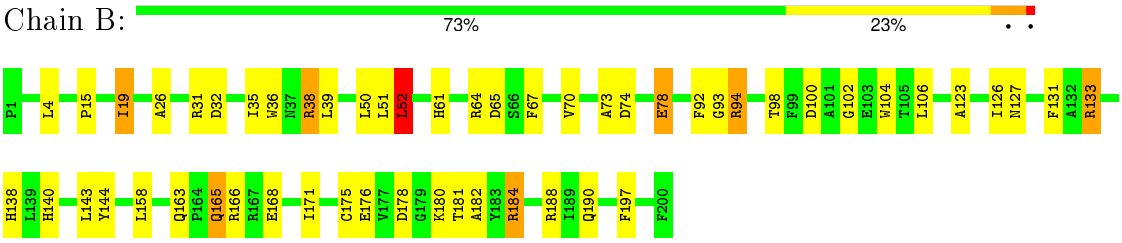
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



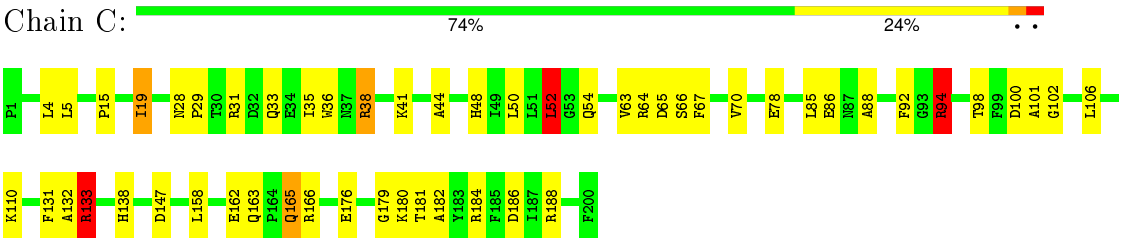
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



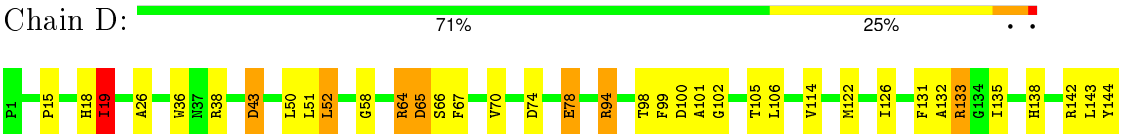
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

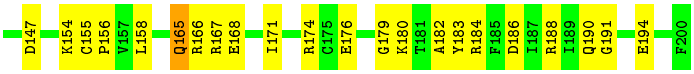
Chain C:



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

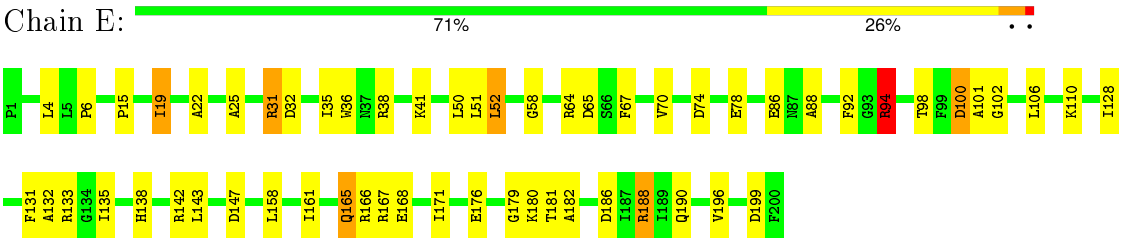
Chain D:





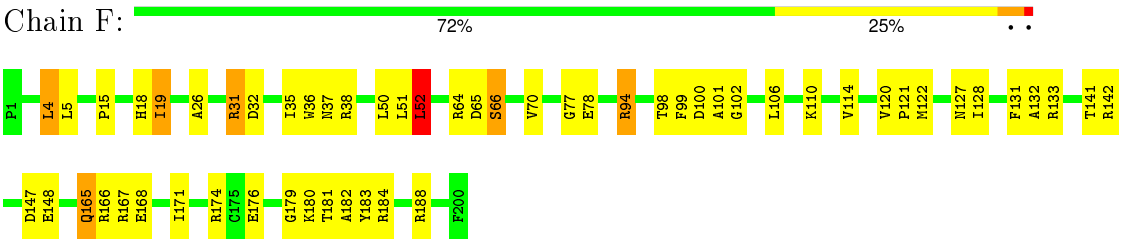
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



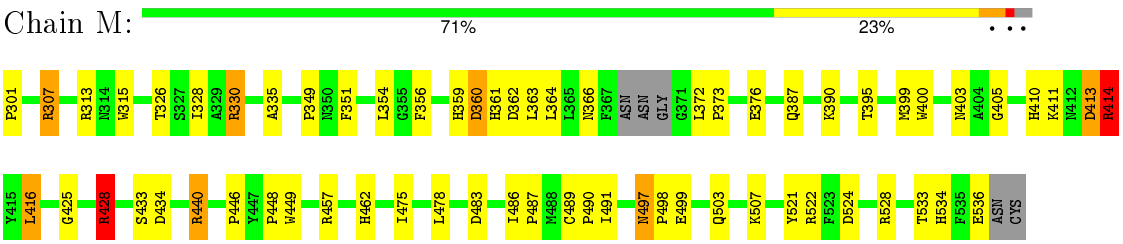
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:



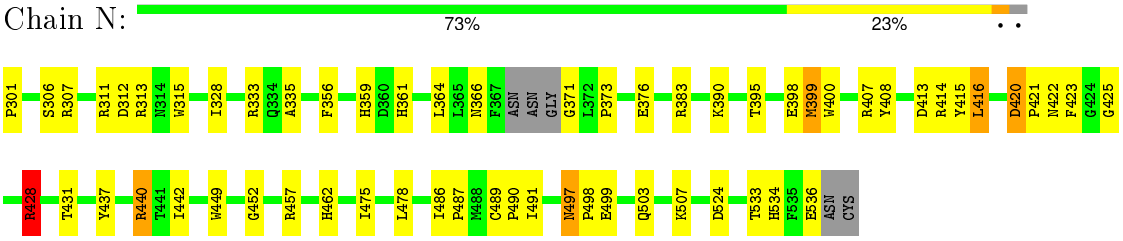
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:



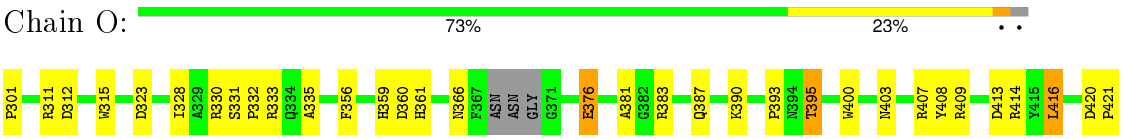
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N:



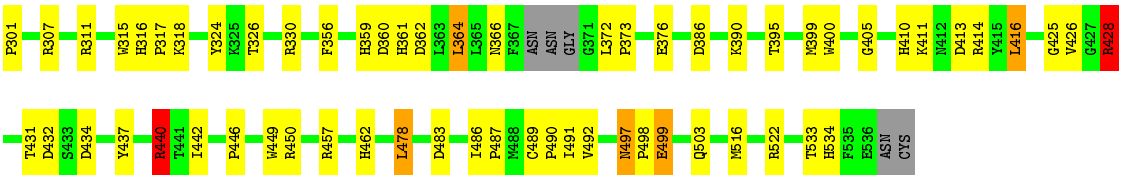
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:



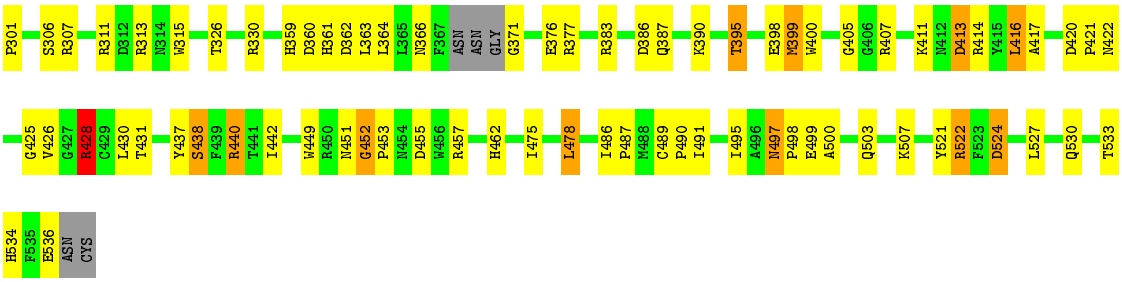
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



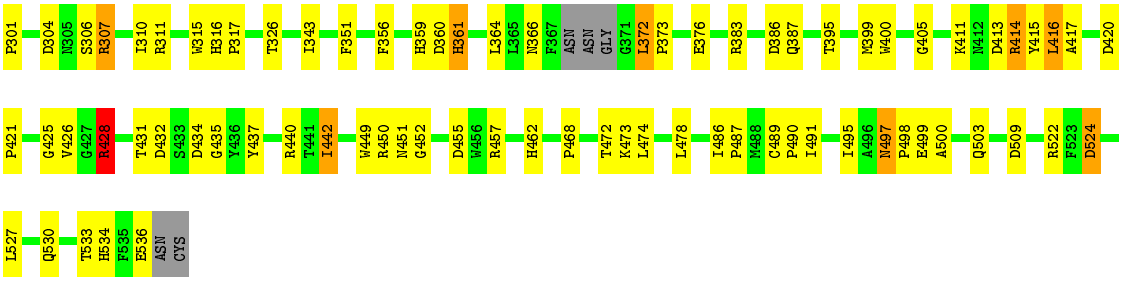
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.60Å 127.50Å 134.30Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.0 (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22014	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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, DHY, BME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.82	0/1611	1.42	20/2195 (0.9%)
1	B	0.85	1/1611 (0.1%)	1.44	19/2195 (0.9%)
1	C	0.85	0/1611	1.35	12/2195 (0.5%)
1	D	0.83	0/1611	1.40	23/2195 (1.0%)
1	E	0.85	0/1611	1.38	15/2195 (0.7%)
1	F	0.91	0/1611	1.54	19/2195 (0.9%)
2	M	0.88	0/1895	1.38	15/2580 (0.6%)
2	N	0.85	0/1895	1.36	13/2580 (0.5%)
2	O	0.88	0/1895	1.40	22/2580 (0.9%)
2	P	0.86	0/1895	1.38	14/2580 (0.5%)
2	Q	0.91	0/1895	1.42	22/2580 (0.9%)
2	R	0.91	0/1895	1.36	16/2580 (0.6%)
All	All	0.87	1/21036 (0.0%)	1.40	210/28650 (0.7%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	ARG	CD-NE	-5.31	1.37	1.46

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	94	ARG	CD-NE-CZ	26.41	160.57	123.60
1	F	94	ARG	CA-CB-CG	16.27	149.21	113.40
2	Q	440	ARG	NE-CZ-NH2	-14.30	113.15	120.30
2	N	440	ARG	NE-CZ-NH2	-13.23	113.68	120.30
2	O	440	ARG	NE-CZ-NH2	-12.81	113.90	120.30
2	P	440	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	D	94	ARG	NE-CZ-NH2	-11.80	114.40	120.30
2	Q	428	ARG	NE-CZ-NH2	-11.19	114.71	120.30
2	R	440	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	B	184	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	Q	330	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	P	440	ARG	NE-CZ-NH1	9.73	125.17	120.30
2	M	440	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	B	133	ARG	NE-CZ-NH2	-9.57	115.52	120.30
2	M	313	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	F	166	ARG	NE-CZ-NH1	9.23	124.91	120.30
1	C	188	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	O	428	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	B	94	ARG	CD-NE-CZ	8.75	135.85	123.60
1	B	94	ARG	CG-CD-NE	8.73	130.13	111.80
1	A	94	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	B	166	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	C	166	ARG	NE-CZ-NH2	-8.30	116.15	120.30
2	R	428	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	Q	428	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	166	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	Q	428	ARG	CD-NE-CZ	8.03	134.84	123.60
2	O	528	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	O	428	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	133	ARG	NE-CZ-NH2	-7.99	116.31	120.30
2	N	457	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	166	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	174	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	38	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	Q	457	ARG	NE-CZ-NH2	-7.87	116.37	120.30
2	Q	524	ASP	CB-CG-OD1	7.86	125.37	118.30
1	E	199	ASP	CB-CG-OD2	7.83	125.35	118.30
2	P	428	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	P	432	ASP	CB-CG-OD1	7.75	125.28	118.30
1	B	188	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	R	428	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	N	313	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	D	133	ARG	NE-CZ-NH2	-7.58	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	184	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	F	142	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	N	524	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	D	166	ARG	NE-CZ-NH2	-7.45	116.57	120.30
2	R	457	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	F	38	ARG	CA-CB-CG	7.29	129.43	113.40
1	D	186	ASP	CB-CG-OD1	7.26	124.84	118.30
2	N	524	ASP	CB-CG-OD1	7.21	124.79	118.30
2	O	457	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	C	52	LEU	CB-CA-C	7.16	123.80	110.20
1	A	186	ASP	CB-CG-OD1	7.10	124.69	118.30
1	F	188	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	31	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	D	133	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	C	166	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	Q	377	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	F	94	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	O	323	ASP	CB-CG-OD1	7.00	124.60	118.30
2	M	414	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	166	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	65	ASP	CB-CG-OD1	6.77	124.40	118.30
2	Q	524	ASP	CB-CG-OD2	-6.76	112.22	118.30
2	M	457	ARG	CD-NE-CZ	6.76	133.06	123.60
1	B	133	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	174	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	188	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	M	428	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	Q	330	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	E	94	ARG	CA-CB-CG	6.50	127.69	113.40
2	Q	311	ARG	NE-CZ-NH2	-6.49	117.05	120.30
2	R	414	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	D	52	LEU	CB-CA-C	6.44	122.43	110.20
2	R	307	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	O	312	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	166	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	R	524	ASP	CB-CG-OD1	6.30	123.97	118.30
2	N	383	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	F	36	TRP	CB-CA-C	6.26	122.92	110.40
2	M	428	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	64	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	E	74	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	52	LEU	CB-CA-C	6.22	122.01	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	186	ASP	CB-CG-OD1	6.21	123.89	118.30
2	N	311	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	P	457	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	O	383	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	R	414	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	R	311	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	R	432	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	184	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	O	333	ARG	NE-CZ-NH2	-6.09	117.26	120.30
2	P	432	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	31	ARG	NE-CZ-NH2	-6.05	117.28	120.30
2	R	509	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	31	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	P	457	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	188	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	Q	360	ASP	CB-CG-OD1	6.01	123.71	118.30
2	O	440	ARG	NH1-CZ-NH2	6.00	126.00	119.40
1	F	94	ARG	CB-CG-CD	5.97	127.11	111.60
1	B	133	ARG	CA-CB-CG	5.96	126.52	113.40
1	E	38	ARG	CD-NE-CZ	-5.94	115.28	123.60
2	O	517	ASP	CB-CG-OD1	5.92	123.63	118.30
1	F	52	LEU	CA-CB-CG	5.92	128.91	115.30
2	Q	413	ASP	CB-CG-OD1	5.91	123.62	118.30
2	P	428	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	166	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	52	LEU	CB-CA-C	5.88	121.38	110.20
2	Q	313	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	188	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	M	524	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	174	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	186	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	142	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	E	167	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	O	428	ARG	CD-NE-CZ	5.75	131.65	123.60
1	D	74	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	31	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	52	LEU	CB-CA-C	5.74	121.10	110.20
2	Q	438	SER	N-CA-CB	5.72	119.09	110.50
2	M	528	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	64	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	Q	360	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	R	361	HIS	CA-CB-CG	-5.67	103.96	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	457	ARG	CD-NE-CZ	5.62	131.47	123.60
2	O	407	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	O	311	ARG	NE-CZ-NH1	-5.61	117.50	120.30
2	M	330	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	36	TRP	CB-CA-C	5.60	121.60	110.40
1	D	188	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	94	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	R	440	ARG	CD-NE-CZ	-5.57	115.81	123.60
1	A	23	LEU	CB-CA-C	5.54	120.73	110.20
1	C	94	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	F	52	LEU	CB-CA-C	5.54	120.73	110.20
1	A	65	ASP	CB-CG-OD1	5.54	123.28	118.30
1	F	166	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	36	TRP	CB-CA-C	5.52	121.44	110.40
2	Q	452	GLY	N-CA-C	-5.51	99.33	113.10
2	R	450	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	P	457	ARG	CD-NE-CZ	5.49	131.29	123.60
1	D	188	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	E	100	ASP	CB-CG-OD2	5.49	123.24	118.30
2	Q	457	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	O	432	ASP	CB-CG-OD1	5.47	123.22	118.30
2	P	457	ARG	CA-CB-CG	5.45	125.40	113.40
2	O	452	GLY	N-CA-C	-5.45	99.47	113.10
1	F	142	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	O	509	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	78	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	A	74	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	A	36	TRP	CB-CA-C	5.40	121.19	110.40
1	D	19	ILE	CB-CA-C	5.38	122.37	111.60
2	N	452	GLY	N-CA-C	-5.38	99.66	113.10
2	O	409	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	E	166	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	141	THR	CA-CB-CG2	5.33	119.87	112.40
1	E	36	TRP	CB-CA-C	5.33	121.06	110.40
2	R	440	ARG	NH1-CZ-NH2	5.33	125.27	119.40
2	O	440	ARG	CD-NE-CZ	-5.32	116.15	123.60
2	N	440	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	D	167	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	52	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	133	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	M	360	ASP	CB-CG-OD1	5.27	123.05	118.30
2	M	521	TYR	CB-CG-CD2	-5.27	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	483	ASP	CB-CG-OD2	5.25	123.03	118.30
1	F	38	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	M	457	ARG	CA-CB-CG	5.24	124.92	113.40
1	A	74	ASP	CB-CG-OD1	5.22	123.00	118.30
2	N	428	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	52	LEU	CA-CB-CG	5.21	127.28	115.30
2	Q	522	ARG	NE-CZ-NH1	-5.21	117.70	120.30
2	O	330	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	F	188	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	P	386	ASP	CB-CA-C	5.19	120.79	110.40
2	M	307	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	74	ASP	CB-CG-OD1	5.18	122.97	118.30
1	E	31	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	Q	440	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	184	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	133	ARG	CA-CB-CG	5.15	124.72	113.40
1	B	31	ARG	CD-NE-CZ	5.14	130.80	123.60
1	E	142	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	P	450	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	D	43	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	174	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	Q	521	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	C	38	ARG	CD-NE-CZ	-5.11	116.44	123.60
2	N	311	ARG	CD-NE-CZ	5.08	130.72	123.60
1	E	52	LEU	CA-CB-CG	5.08	126.99	115.30
1	F	31	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	38	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	O	376	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	B	175	CYS	CA-CB-SG	5.05	123.08	114.00
2	O	457	ARG	CA-CB-CG	5.05	124.50	113.40
2	M	413	ASP	CB-CG-OD1	5.04	122.84	118.30
2	P	483	ASP	CB-CG-OD2	5.04	122.84	118.30
2	Q	522	ARG	CD-NE-CZ	-5.03	116.55	123.60
1	A	31	ARG	CD-NE-CZ	5.03	130.65	123.60
1	B	184	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	178	ASP	CB-CG-OD1	5.03	122.83	118.30
2	N	420	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	78	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	F	94	ARG	CG-CD-NE	5.02	122.34	111.80
2	N	312	ASP	CB-CG-OD1	5.01	122.81	118.30
2	P	311	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	44	0
1	B	1571	0	1499	43	0
1	C	1571	0	1499	43	0
1	D	1571	0	1499	44	0
1	E	1571	0	1499	49	0
1	F	1571	0	1499	49	0
2	M	1840	0	1793	66	0
2	N	1840	0	1793	48	0
2	O	1840	0	1793	47	0
2	P	1840	0	1793	52	0
2	Q	1840	0	1793	70	0
2	R	1840	0	1793	77	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	1	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	3	0
4	R	4	0	5	1	0
5	M	24	0	10	8	0
5	N	24	0	10	10	0
5	O	24	0	10	7	0
5	P	24	0	10	8	0
5	Q	24	0	12	11	0
5	R	24	0	10	8	0
6	A	80	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	79	0	0	0	0
6	C	81	0	0	0	0
6	D	82	0	0	0	0
6	E	80	0	0	1	0
6	F	79	0	0	1	0
6	M	150	0	0	6	0
6	N	152	0	0	2	0
6	O	147	0	0	5	0
6	P	145	0	0	4	0
6	Q	149	0	0	6	0
6	R	150	0	0	3	0
All	All	22014	0	19844	572	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (572) 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)
2:N:491:ILE:HD11	5:N:550[A]:DHY:H72	1.23	1.17
1:E:165:GLN:NE2	1:E:165:GLN:H	1.50	1.08
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.27	1.06
1:E:165:GLN:N	1:E:165:GLN:HE21	1.55	1.03
2:P:491:ILE:HD11	5:P:550[A]:DHY:H72	1.43	0.99
2:O:462:HIS:CE1	5:O:550[B]:DHY:O4	2.15	0.98
2:Q:491:ILE:HD11	5:Q:550[A]:DHY:H72	1.42	0.98
1:B:165:GLN:HE21	1:B:165:GLN:H	1.05	0.97
1:B:165:GLN:NE2	1:B:165:GLN:H	1.64	0.95
2:M:491:ILE:HD11	5:M:550[A]:DHY:H72	1.47	0.94
2:R:491:ILE:HD11	5:R:550[A]:DHY:H72	1.49	0.93
2:N:462:HIS:CE1	5:N:550[B]:DHY:O4	2.21	0.93
2:R:497:ASN:ND2	2:R:499:GLU:H	1.67	0.92
2:R:497:ASN:HD22	2:R:499:GLU:H	1.20	0.90
2:N:449:TRP:CE3	5:N:550[B]:DHY:H72	2.07	0.90
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.03	0.88
1:D:165:GLN:H	1:D:165:GLN:HE21	1.21	0.88
1:E:98:THR:HB	1:E:100:ASP:OD1	1.74	0.88
2:Q:462:HIS:CE1	5:Q:550[B]:DHY:O4	2.27	0.87
2:O:491:ILE:HD11	5:O:550[A]:DHY:H72	1.55	0.87
2:R:361:HIS:H	2:R:361:HIS:CD2	1.93	0.86
2:O:462:HIS:HE1	5:O:550[B]:DHY:O4	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:449:TRP:CE3	5:R:550[A]:DHY:H71	2.11	0.86
2:Q:462:HIS:HE1	5:Q:550[B]:DHY:O4	1.59	0.85
2:Q:449:TRP:CE3	5:Q:550[A]:DHY:H71	2.11	0.85
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.92	0.85
1:C:64:ARG:NH1	1:C:100:ASP:O	2.10	0.84
2:M:497:ASN:ND2	2:M:499:GLU:H	1.75	0.83
2:N:491:ILE:CD1	5:N:550[A]:DHY:H72	2.06	0.83
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.61	0.83
1:F:64:ARG:NH1	1:F:100:ASP:O	2.11	0.83
2:R:462:HIS:CE1	5:R:550[B]:DHY:O4	2.32	0.82
2:Q:449:TRP:CE3	5:Q:550[B]:DHY:H72	2.15	0.81
2:R:361:HIS:H	2:R:361:HIS:HD2	1.29	0.81
1:D:64:ARG:NH1	1:D:100:ASP:O	2.14	0.80
2:M:449:TRP:CE3	5:M:550[B]:DHY:H72	2.17	0.80
1:A:67:PHE:CZ	1:A:94:ARG:HD3	2.17	0.80
2:Q:491:ILE:CD1	5:Q:550[A]:DHY:H72	2.12	0.79
2:M:497:ASN:HD22	2:M:499:GLU:H	1.26	0.79
2:R:449:TRP:CE3	5:R:550[B]:DHY:H72	2.17	0.79
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.48	0.79
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.48	0.78
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.63	0.78
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.83	0.78
2:O:449:TRP:CE3	5:O:550[B]:DHY:H72	2.18	0.78
2:M:462:HIS:CE1	5:M:550[B]:DHY:O4	2.35	0.78
2:R:536:GLU:HB2	6:R:1301:HOH:O	1.84	0.77
2:M:449:TRP:CE3	5:M:550[A]:DHY:H71	2.20	0.77
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.83	0.77
1:A:98:THR:HB	1:A:100:ASP:OD1	1.84	0.76
2:P:491:ILE:CD1	5:P:550[A]:DHY:H72	2.16	0.76
2:P:449:TRP:CE3	5:P:550[B]:DHY:H72	2.20	0.76
1:C:98:THR:HB	1:C:100:ASP:OD1	1.86	0.76
2:P:361:HIS:CD2	2:P:361:HIS:H	2.04	0.76
2:O:449:TRP:CE3	5:O:550[A]:DHY:H71	2.20	0.76
2:R:491:ILE:CD1	5:R:550[A]:DHY:H72	2.16	0.75
2:N:390:LYS:HE2	6:N:726:HOH:O	1.87	0.75
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.03	0.74
2:Q:462:HIS:CE1	5:Q:550[B]:DHY:HO4	2.04	0.74
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.52	0.74
2:N:491:ILE:HD11	5:N:550[A]:DHY:C7	2.11	0.74
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.53	0.74
1:B:98:THR:HB	1:B:100:ASP:OD1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:HZ	1:A:94:ARG:HD3	1.49	0.74
1:F:165:GLN:NE2	1:F:165:GLN:H	1.86	0.73
2:R:462:HIS:HE1	5:R:550[B]:DHY:O4	1.68	0.73
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.70	0.73
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.52	0.73
1:D:98:THR:HB	1:D:100:ASP:OD1	1.89	0.73
1:B:176:GLU:HG3	1:B:180:LYS:O	1.88	0.73
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.24	0.73
2:M:390:LYS:HD3	6:M:640:HOH:O	1.89	0.72
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.72	0.72
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.19	0.72
1:D:165:GLN:H	1:D:165:GLN:NE2	1.87	0.72
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.23	0.72
1:F:165:GLN:H	1:F:165:GLN:HE21	1.38	0.71
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.20	0.71
1:B:165:GLN:N	1:B:165:GLN:HE21	1.85	0.71
1:F:176:GLU:HG3	1:F:180:LYS:O	1.91	0.71
1:E:64:ARG:NH1	1:E:100:ASP:O	2.23	0.70
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.27	0.70
2:M:491:ILE:CD1	5:M:550[A]:DHY:H72	2.20	0.70
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.73	0.70
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.72	0.70
1:C:165:GLN:H	1:C:165:GLN:NE2	1.90	0.69
1:F:98:THR:HB	1:F:100:ASP:OD1	1.92	0.69
2:M:361:HIS:H	2:M:361:HIS:CD2	2.10	0.68
2:O:491:ILE:CD1	5:O:550[A]:DHY:H72	2.24	0.68
2:Q:438:SER:O	4:Q:601:BME:H22	1.94	0.68
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.75	0.68
1:A:176:GLU:HA	1:A:180:LYS:O	1.94	0.67
2:P:361:HIS:HD2	2:P:361:HIS:H	1.41	0.67
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.59	0.67
2:Q:390:LYS:HD3	6:Q:992:HOH:O	1.95	0.67
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.29	0.67
2:O:497:ASN:HD22	2:O:499:GLU:H	1.41	0.67
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.95	0.67
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.43	0.67
2:Q:390:LYS:HE2	6:Q:1109:HOH:O	1.93	0.66
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.95	0.66
1:B:78:GLU:HG2	2:N:301:PRO:CB	2.26	0.66
2:P:449:TRP:CE3	5:P:550[A]:DHY:H71	2.30	0.66
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:536:GLU:HB2	6:Q:1072:HOH:O	1.95	0.66
2:N:361:HIS:H	2:N:361:HIS:CD2	2.14	0.65
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.43	0.65
2:N:449:TRP:CE3	5:N:550[A]:DHY:H71	2.32	0.65
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.79	0.65
1:E:98:THR:O	1:E:102:GLY:HA2	1.97	0.65
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.31	0.65
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.95	0.65
2:R:497:ASN:HD22	2:R:497:ASN:C	2.00	0.64
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.77	0.64
1:B:78:GLU:HG2	2:N:301:PRO:CG	2.28	0.64
2:Q:405:GLY:HA3	6:Q:996:HOH:O	1.98	0.64
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.63	0.64
2:R:405:GLY:HA3	6:R:1225:HOH:O	1.98	0.64
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.80	0.63
2:O:497:ASN:ND2	2:O:499:GLU:H	1.96	0.63
1:F:15:PRO:HB3	1:F:133:ARG:HD2	1.80	0.63
2:Q:449:TRP:CZ3	5:Q:550[A]:DHY:H71	2.33	0.63
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.81	0.63
2:Q:376:GLU:O	2:Q:442:ILE:HA	1.99	0.63
2:P:462:HIS:HE1	5:P:550[B]:DHY:O4	1.71	0.63
2:O:361:HIS:CD2	2:O:361:HIS:H	2.15	0.63
2:M:522:ARG:NH1	6:M:664:HOH:O	2.32	0.63
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.80	0.62
1:F:50:LEU:O	1:F:182:ALA:HA	1.99	0.62
2:R:400:TRP:HA	2:R:425:GLY:O	1.99	0.62
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.46	0.62
1:E:176:GLU:HA	1:E:180:LYS:O	2.00	0.62
2:P:376:GLU:O	2:P:442:ILE:HA	1.99	0.62
1:D:78:GLU:HG2	2:P:301:PRO:HB3	1.82	0.62
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.18	0.62
1:A:162:GLU:OE2	1:C:133:ARG:NH2	2.33	0.62
1:C:176:GLU:OE2	1:C:179:GLY:HA2	1.98	0.62
2:P:497:ASN:HD22	2:P:499:GLU:H	1.44	0.62
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	1.98	0.62
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.79	0.62
2:P:405:GLY:HA3	6:P:647:HOH:O	1.99	0.62
2:R:356:PHE:HD1	2:R:428:ARG:HD3	1.64	0.62
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.47	0.62
1:B:133:ARG:NH2	1:C:162:GLU:OE2	2.33	0.62
1:D:78:GLU:HG2	2:P:301:PRO:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.00	0.61
2:R:416:LEU:HD23	2:R:416:LEU:C	2.20	0.61
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.30	0.61
1:D:100:ASP:CG	1:D:101:ALA:H	2.04	0.61
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.83	0.60
2:N:462:HIS:HE1	5:N:550[B]:DHY:O4	1.70	0.60
1:F:78:GLU:HG2	2:R:301:PRO:CB	2.31	0.60
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.05	0.60
2:P:376:GLU:OE1	6:P:639:HOH:O	2.15	0.60
1:C:78:GLU:HG2	2:O:301:PRO:HB3	1.84	0.60
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.16	0.60
2:M:361:HIS:HD2	2:M:361:HIS:H	1.49	0.60
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.83	0.60
1:D:176:GLU:HG3	1:D:180:LYS:O	2.01	0.60
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.37	0.59
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.84	0.59
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.32	0.59
2:Q:371:GLY:HA3	2:Q:422:ASN:ND2	2.17	0.59
2:R:497:ASN:HD22	2:R:498:PRO:N	2.00	0.59
2:O:376:GLU:O	2:O:442:ILE:HA	2.02	0.59
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.38	0.59
2:R:416:LEU:HD23	2:R:417:ALA:N	2.18	0.59
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.36	0.59
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.01	0.59
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.17	0.58
2:M:497:ASN:HD22	2:M:498:PRO:N	2.00	0.58
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.38	0.58
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.23	0.58
1:C:165:GLN:H	1:C:165:GLN:HE21	1.52	0.58
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.85	0.58
2:O:390:LYS:HD2	6:O:647:HOH:O	2.03	0.58
1:F:168:GLU:HA	1:F:171:ILE:HD13	1.85	0.58
1:F:19:ILE:O	2:R:426:VAL:HG21	2.04	0.58
2:R:497:ASN:HD22	2:R:499:GLU:N	1.97	0.57
1:B:98:THR:O	1:B:102:GLY:HA2	2.04	0.57
1:B:176:GLU:HG3	1:B:180:LYS:C	2.24	0.57
2:O:403:ASN:HB2	6:O:612:HOH:O	2.03	0.57
2:N:449:TRP:CZ3	5:N:550[A]:DHY:H71	2.40	0.57
2:Q:411:LYS:O	2:Q:414:ARG:NH1	2.37	0.57
1:D:19:ILE:O	2:P:426:VAL:HG21	2.03	0.57
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:HIS:HE1	5:M:550[B]:DHY:O4	1.78	0.57
2:R:449:TRP:CZ3	5:R:550[A]:DHY:H71	2.39	0.57
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.70	0.57
2:Q:522:ARG:NH1	6:Q:1029:HOH:O	2.37	0.57
1:F:133:ARG:HG2	2:R:326:THR:HG21	1.87	0.57
1:F:131:PHE:O	1:F:132:ALA:HB2	2.04	0.57
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.87	0.57
2:R:361:HIS:N	2:R:361:HIS:CD2	2.65	0.56
2:O:416:LEU:C	2:O:416:LEU:HD23	2.25	0.56
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.86	0.56
2:Q:361:HIS:ND1	4:Q:601:BME:H21	2.20	0.56
1:B:78:GLU:HG2	2:N:301:PRO:HB3	1.86	0.56
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.03	0.56
2:N:497:ASN:HD22	2:N:499:GLU:H	1.53	0.56
2:P:486:ILE:HB	2:P:487:PRO:HD3	1.86	0.56
2:M:390:LYS:HE2	6:M:717:HOH:O	2.05	0.56
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.36	0.56
1:C:78:GLU:HG2	2:O:301:PRO:CB	2.35	0.56
2:Q:306:SER:OG	2:Q:530:GLN:NE2	2.21	0.56
1:D:132:ALA:HB3	1:D:135:ILE:HD12	1.87	0.56
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.88	0.56
2:M:449:TRP:CZ3	5:M:550[A]:DHY:H71	2.40	0.56
2:P:413:ASP:O	2:P:414:ARG:NH1	2.39	0.56
2:M:497:ASN:HD22	2:M:497:ASN:C	2.10	0.55
2:Q:363:LEU:N	2:Q:363:LEU:HD12	2.21	0.55
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	2.06	0.55
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.06	0.55
1:E:98:THR:OG1	1:E:102:GLY:N	2.39	0.55
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.55
1:C:131:PHE:O	1:C:132:ALA:HB2	2.05	0.55
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.89	0.55
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.88	0.55
2:R:497:ASN:ND2	2:R:499:GLU:N	2.49	0.55
1:D:176:GLU:OE2	1:D:179:GLY:HA2	2.06	0.55
1:F:100:ASP:CG	1:F:101:ALA:H	2.10	0.55
2:P:400:TRP:HA	2:P:425:GLY:O	2.07	0.55
1:A:114:VAL:HG23	1:A:122:MET:CE	2.37	0.55
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.54	0.55
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.41	0.55
1:C:98:THR:O	1:C:102:GLY:HA2	2.07	0.55
1:A:100:ASP:CG	1:A:101:ALA:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.95	0.54
1:D:98:THR:O	1:D:102:GLY:HA2	2.08	0.54
1:D:15:PRO:HB3	1:D:133:ARG:HD2	1.90	0.54
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.43	0.54
1:F:32:ASP:HB2	6:F:1348:HOH:O	2.05	0.54
2:P:307:ARG:CG	2:P:533:THR:HG22	2.36	0.54
2:M:478:LEU:C	2:M:478:LEU:HD23	2.28	0.54
2:N:361:HIS:HD2	2:N:361:HIS:H	1.55	0.54
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.54
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.23	0.54
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.54
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.21	0.54
1:D:165:GLN:N	1:D:165:GLN:HE21	2.00	0.53
1:B:35:ILE:HG21	1:B:92:PHE:CE2	2.42	0.53
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.72	0.53
2:O:449:TRP:CZ3	5:O:550[A]:DHY:H71	2.44	0.53
2:R:451:ASN:HB3	2:R:455:ASP:OD2	2.07	0.53
2:Q:462:HIS:CE1	5:Q:550[A]:DHY:O3	2.62	0.53
1:A:64:ARG:NH1	1:A:100:ASP:O	2.41	0.53
1:E:100:ASP:CG	1:E:101:ALA:H	2.12	0.53
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.90	0.53
1:F:110:LYS:HE2	1:F:148:GLU:OE2	2.08	0.53
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.42	0.53
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.55	0.53
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.74	0.53
2:Q:453:PRO:CB	2:R:310:ILE:HD12	2.35	0.53
1:D:18:HIS:CE1	1:D:99:PHE:CE1	2.96	0.52
1:A:176:GLU:HG3	1:A:180:LYS:O	2.09	0.52
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.77	0.52
2:R:468:PRO:HD2	2:R:472:THR:HG21	1.92	0.52
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.39	0.52
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.90	0.52
2:M:536:GLU:HB2	6:M:696:HOH:O	2.09	0.52
1:F:100:ASP:N	1:F:100:ASP:OD1	2.39	0.52
2:N:400:TRP:HA	2:N:425:GLY:O	2.09	0.52
1:A:50:LEU:O	1:A:182:ALA:HA	2.08	0.52
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.25	0.52
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.92	0.52
2:M:413:ASP:C	2:M:414:ARG:HD2	2.30	0.52
2:M:399:MET:HA	2:M:462:HIS:O	2.10	0.52
1:E:176:GLU:HG3	1:E:180:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:GLY:O	1:D:194:GLU:HB2	2.10	0.52
1:A:114:VAL:HG23	1:A:122:MET:HE2	1.92	0.52
2:O:413:ASP:O	2:O:414:ARG:NH1	2.41	0.52
1:C:44:ALA:O	1:C:48:HIS:NE2	2.29	0.52
2:N:376:GLU:O	2:N:442:ILE:HA	2.10	0.51
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.46	0.51
1:D:18:HIS:CE1	1:D:99:PHE:HE1	2.28	0.51
2:M:416:LEU:HD23	2:M:416:LEU:C	2.31	0.51
1:F:180:LYS:HG2	1:F:181:THR:N	2.25	0.51
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.92	0.51
2:Q:453:PRO:HB2	2:R:310:ILE:CD1	2.38	0.51
1:C:176:GLU:HA	1:C:180:LYS:O	2.10	0.51
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.51
1:D:114:VAL:HG23	1:D:122:MET:CE	2.41	0.51
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.33	0.51
1:D:114:VAL:HG23	1:D:122:MET:HE2	1.93	0.51
1:F:77:GLY:O	1:F:114:VAL:HG12	2.11	0.51
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.74	0.51
2:N:413:ASP:O	2:N:414:ARG:NH1	2.44	0.51
1:E:94:ARG:NH2	2:Q:398:GLU:OE2	2.44	0.50
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.26	0.50
2:R:359:HIS:O	2:R:366:ASN:HB3	2.11	0.50
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.27	0.50
2:R:399:MET:HA	2:R:462:HIS:O	2.12	0.50
1:C:5:LEU:O	2:O:387:GLN:HG2	2.10	0.50
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.32	0.50
1:C:41:LYS:NZ	1:C:86:GLU:O	2.44	0.50
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.47	0.50
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.47	0.50
2:P:522:ARG:NH1	6:P:666:HOH:O	2.44	0.50
1:F:70:VAL:HG12	1:F:128:ILE:HG12	1.92	0.50
2:P:416:LEU:HD23	2:P:416:LEU:C	2.31	0.50
2:Q:371:GLY:HA3	2:Q:422:ASN:CG	2.32	0.49
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.10	0.49
2:O:359:HIS:O	2:O:366:ASN:HB3	2.13	0.49
2:M:328:ILE:HD12	2:N:335:ALA:HB2	1.94	0.49
2:O:400:TRP:HA	2:O:425:GLY:O	2.12	0.49
2:N:449:TRP:CE3	5:N:550[B]:DHY:C7	2.89	0.49
2:N:306:SER:O	2:N:307:ARG:NH1	2.45	0.49
2:Q:407:ARG:HD3	2:Q:417:ALA:O	2.12	0.49
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.47	0.49
2:N:371:GLY:HA3	2:N:422:ASN:CG	2.33	0.49
1:B:51:LEU:HD11	1:B:126:ILE:HD12	1.93	0.49
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.48	0.49
2:Q:462:HIS:HE1	5:Q:550[A]:DHY:O3	1.95	0.49
1:C:98:THR:OG1	1:C:102:GLY:N	2.45	0.49
1:F:98:THR:OG1	1:F:102:GLY:N	2.42	0.49
1:A:67:PHE:CE1	1:A:94:ARG:HD3	2.48	0.49
1:E:133:ARG:HG2	2:Q:326:THR:HG21	1.93	0.49
1:C:100:ASP:CG	1:C:101:ALA:H	2.16	0.48
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.14	0.48
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.95	0.48
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.49	0.48
1:A:180:LYS:HG2	1:A:181:THR:N	2.28	0.48
1:D:66:SER:HA	1:D:132:ALA:HB2	1.95	0.48
2:N:536:GLU:HB2	6:N:704:HOH:O	2.12	0.48
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.44	0.48
2:R:306:SER:CB	2:R:530:GLN:HE21	2.25	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.49	0.48
2:P:478:LEU:C	2:P:478:LEU:HD23	2.33	0.48
1:D:131:PHE:O	1:D:132:ALA:HB2	2.14	0.48
2:N:359:HIS:O	2:N:366:ASN:HB3	2.14	0.48
1:B:50:LEU:O	1:B:182:ALA:HA	2.14	0.48
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.96	0.48
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.96	0.48
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.73	0.48
1:C:66:SER:HA	1:C:132:ALA:HB2	1.96	0.48
1:B:52:LEU:HD21	1:B:184:ARG:NH1	2.27	0.48
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.96	0.47
2:P:489:CYS:HB3	2:P:492:VAL:HB	1.96	0.47
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.56	0.47
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.97	0.47
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.61	0.47
1:B:94:ARG:NH2	2:N:398:GLU:OE2	2.46	0.47
1:D:176:GLU:HA	1:D:180:LYS:O	2.14	0.47
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.15	0.47
2:R:386:ASP:HA	2:R:527:LEU:O	2.13	0.47
2:P:497:ASN:ND2	2:P:499:GLU:H	2.11	0.47
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.14	0.47
2:O:497:ASN:HD22	2:O:497:ASN:C	2.18	0.47
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:399:MET:HA	2:Q:462:HIS:O	2.15	0.47
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.80	0.47
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.15	0.47
2:N:431:THR:HG22	2:N:437:TYR:HB3	1.97	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.81	0.47
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.49	0.47
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.15	0.47
1:C:19:ILE:O	2:O:426:VAL:HG21	2.15	0.47
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.96	0.47
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.97	0.47
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.95	0.47
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.97	0.47
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.50	0.47
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.96	0.47
1:E:78:GLU:HG2	2:Q:301:PRO:HB3	1.97	0.47
2:N:478:LEU:C	2:N:478:LEU:HD23	2.36	0.47
1:D:51:LEU:O	1:D:105:THR:HA	2.15	0.46
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.47	0.46
2:O:486:ILE:N	2:O:487:PRO:HD2	2.31	0.46
2:O:361:HIS:HD2	6:O:704:HOH:O	1.98	0.46
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.28	0.46
2:N:399:MET:HA	2:N:462:HIS:O	2.16	0.46
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.98	0.46
1:E:188:ARG:HH11	1:E:188:ARG:HG3	1.80	0.46
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.96	0.46
1:A:165:GLN:H	1:A:165:GLN:CD	2.18	0.46
2:O:356:PHE:CD1	2:O:428:ARG:CD	2.98	0.46
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.76	0.46
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.78	0.46
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.97	0.46
2:P:449:TRP:CZ3	5:P:550[A]:DHY:H71	2.51	0.46
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.46
2:Q:390:LYS:CD	6:Q:992:HOH:O	2.59	0.46
2:N:413:ASP:C	2:N:414:ARG:HD2	2.36	0.46
2:N:420:ASP:HA	2:N:421:PRO:HD2	1.79	0.46
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.16	0.46
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.31	0.46
1:E:131:PHE:O	1:E:132:ALA:HB2	2.16	0.46
2:M:414:ARG:HD2	2:M:414:ARG:N	2.32	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.31	0.46
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.14	0.45
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.98	0.45
1:B:51:LEU:HD11	1:B:126:ILE:CD1	2.46	0.45
1:E:161:ILE:HD13	1:E:196:VAL:HG21	1.99	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.37	0.45
1:F:114:VAL:HG23	1:F:122:MET:CE	2.46	0.45
2:O:413:ASP:C	2:O:414:ARG:HD2	2.37	0.45
2:R:411:LYS:O	2:R:414:ARG:NH1	2.50	0.45
1:E:180:LYS:CG	1:E:181:THR:N	2.80	0.45
1:C:78:GLU:CG	2:O:301:PRO:HG3	2.46	0.45
2:N:371:GLY:HA3	2:N:422:ASN:ND2	2.32	0.45
1:B:143:LEU:HD23	1:B:143:LEU:C	2.37	0.45
1:A:64:ARG:NE	6:A:219:HOH:O	2.44	0.45
1:B:64:ARG:NH1	1:B:100:ASP:O	2.50	0.45
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.83	0.45
2:N:497:ASN:ND2	2:N:499:GLU:H	2.13	0.45
2:M:448:PRO:HB2	2:P:516:MET:HA	1.98	0.45
1:C:100:ASP:OD1	1:C:100:ASP:N	2.35	0.45
1:F:19:ILE:O	2:R:426:VAL:CG2	2.65	0.45
1:C:19:ILE:CD1	2:O:408:TYR:HD2	2.30	0.45
2:R:376:GLU:O	2:R:442:ILE:HA	2.17	0.45
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.33	0.45
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.17	0.44
2:R:522:ARG:NH1	6:R:1258:HOH:O	2.48	0.44
2:R:413:ASP:C	2:R:414:ARG:HD2	2.37	0.44
2:P:431:THR:HG22	2:P:437:TYR:HB3	1.99	0.44
2:M:449:TRP:CD2	5:M:550[B]:DHY:H72	2.52	0.44
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.16	0.44
1:B:52:LEU:HD22	1:B:52:LEU:C	2.38	0.44
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.99	0.44
2:R:431:THR:HG22	2:R:437:TYR:HB3	2.00	0.44
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.80	0.44
1:A:92:PHE:CG	2:M:349:PRO:HG3	2.53	0.44
2:O:361:HIS:CD2	6:O:704:HOH:O	2.71	0.44
2:R:522:ARG:HH21	2:R:524:ASP:CG	2.20	0.44
2:N:373:PRO:HB3	2:N:423:PHE:HB2	1.99	0.44
1:C:50:LEU:O	1:C:182:ALA:HA	2.17	0.44
2:M:354:LEU:HD23	2:M:356:PHE:CE1	2.52	0.44
2:M:361:HIS:CG	4:M:601:BME:H21	2.53	0.44
2:O:497:ASN:HD22	2:O:498:PRO:N	2.15	0.44
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:383:ARG:N	2:Q:524:ASP:OD1	2.47	0.44
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.82	0.44
1:F:110:LYS:CE	1:F:148:GLU:OE2	2.66	0.44
2:R:497:ASN:ND2	2:R:497:ASN:C	2.71	0.44
1:D:98:THR:OG1	1:D:102:GLY:N	2.46	0.44
2:O:361:HIS:CG	4:O:601:BME:H21	2.53	0.44
2:P:316:HIS:HB3	2:P:317:PRO:HD2	2.00	0.44
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.90	0.44
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.17	0.44
2:P:324:TYR:OH	5:P:550[A]:DHY:O1	2.23	0.43
2:Q:449:TRP:CD2	5:Q:550[B]:DHY:H72	2.51	0.43
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.45	0.43
1:B:180:LYS:HG2	1:B:181:THR:N	2.33	0.43
1:F:120:VAL:HA	1:F:121:PRO:HD3	1.84	0.43
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.78	0.43
1:B:140:HIS:O	1:B:197:PHE:HA	2.18	0.43
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.84	0.43
2:P:413:ASP:C	2:P:414:ARG:HD2	2.38	0.43
6:E:242:HOH:O	2:Q:426:VAL:HG21	2.18	0.43
1:B:70:VAL:HG21	1:B:106:LEU:HD21	2.00	0.43
2:M:362:ASP:OD2	2:M:440:ARG:NH1	2.50	0.43
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.92	0.43
1:C:63:VAL:HG12	1:C:66:SER:HB3	2.00	0.43
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.53	0.43
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.43
2:R:449:TRP:CD2	5:R:550[B]:DHY:H72	2.52	0.43
2:M:405:GLY:HA3	6:M:643:HOH:O	2.17	0.43
1:E:6:PRO:HG2	2:Q:503:GLN:NE2	2.34	0.43
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.54	0.43
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.54	0.43
1:A:35:ILE:CD1	2:M:351:PHE:CE1	3.02	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.00	0.43
2:N:486:ILE:HB	2:N:487:PRO:HD3	2.00	0.43
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.39	0.43
2:M:335:ALA:HB2	2:O:328:ILE:HD12	2.01	0.43
2:N:449:TRP:CD2	5:N:550[B]:DHY:H72	2.51	0.43
1:A:165:GLN:H	1:A:165:GLN:NE2	2.17	0.43
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.74	0.43
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.18	0.43
1:E:143:LEU:HD23	1:E:143:LEU:C	2.38	0.43
2:M:497:ASN:ND2	2:M:499:GLU:N	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:O	1:A:102:GLY:HA2	2.19	0.43
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.33	0.43
2:R:372:LEU:HA	2:R:372:LEU:HD12	1.84	0.43
1:E:180:LYS:HG2	1:E:181:THR:N	2.34	0.42
2:R:437:TYR:C	2:R:437:TYR:CD1	2.93	0.42
2:M:446:PRO:HD2	2:P:376:GLU:HG2	2.00	0.42
1:D:78:GLU:HG2	2:P:301:PRO:HG3	2.00	0.42
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.19	0.42
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.54	0.42
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.54	0.42
2:R:451:ASN:HB3	2:R:452:GLY:H	1.67	0.42
1:B:70:VAL:HA	1:B:127:ASN:O	2.20	0.42
1:F:4:LEU:HB3	2:R:387:GLN:HB3	2.00	0.42
1:E:100:ASP:OD1	1:E:100:ASP:N	2.52	0.42
1:F:174:ARG:HE	1:F:181:THR:HG23	1.85	0.42
1:F:37:ASN:HB2	1:F:106:LEU:HD12	2.01	0.42
1:D:50:LEU:O	1:D:182:ALA:HA	2.19	0.42
1:E:165:GLN:H	1:E:165:GLN:HE21	0.69	0.42
2:P:449:TRP:CD2	5:P:550[B]:DHY:H72	2.54	0.42
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.89	0.42
2:M:411:LYS:O	2:M:414:ARG:NH1	2.52	0.42
1:E:133:ARG:HH11	1:E:133:ARG:HD3	1.62	0.42
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.73	0.42
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.00	0.42
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.80	0.42
2:M:400:TRP:HA	2:M:425:GLY:O	2.19	0.42
2:P:362:ASP:OD2	2:P:440:ARG:NH1	2.52	0.42
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.44	0.42
2:R:473:LYS:HD2	2:R:474:LEU:N	2.35	0.42
1:F:70:VAL:HG21	1:F:106:LEU:HD21	2.02	0.42
1:A:4:LEU:HB3	2:M:387:GLN:HB3	2.02	0.42
1:A:63:VAL:HG13	2:M:330:ARG:CZ	2.50	0.42
1:C:158:LEU:HA	1:C:158:LEU:HD12	1.93	0.42
2:Q:451:ASN:HB3	2:Q:452:GLY:H	1.69	0.42
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.94	0.42
1:F:176:GLU:HG3	1:F:180:LYS:C	2.40	0.42
1:E:188:ARG:CG	1:E:188:ARG:HH11	2.33	0.42
2:O:395:THR:O	2:O:430:LEU:HA	2.19	0.42
2:R:361:HIS:ND1	4:R:601:BME:H21	2.35	0.41
1:D:19:ILE:HG22	1:D:26:ALA:HB1	2.02	0.41
1:F:51:LEU:HD23	1:F:183:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LEU:O	1:E:182:ALA:HA	2.20	0.41
2:P:326:THR:HG22	2:P:330:ARG:HD2	2.01	0.41
1:F:167:ARG:O	1:F:171:ILE:HD12	2.20	0.41
2:M:416:LEU:CD2	2:M:416:LEU:C	2.88	0.41
1:E:70:VAL:HG12	1:E:128:ILE:HG12	2.02	0.41
2:R:383:ARG:HA	2:R:435:GLY:O	2.20	0.41
1:E:41:LYS:HZ2	1:E:86:GLU:C	2.23	0.41
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.35	0.41
2:O:381:ALA:O	2:O:522:ARG:HA	2.20	0.41
2:Q:522:ARG:HH11	2:Q:522:ARG:HD3	1.56	0.41
2:P:411:LYS:O	2:P:414:ARG:NH1	2.53	0.41
2:N:328:ILE:HD12	2:O:335:ALA:HB2	2.03	0.41
1:E:22:ALA:O	1:E:25:ALA:HB3	2.20	0.41
1:D:19:ILE:HG21	2:P:410:HIS:HB2	2.03	0.41
2:M:359:HIS:O	2:M:366:ASN:HB3	2.21	0.41
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.83	0.41
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.76	0.41
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.54	0.41
1:D:143:LEU:HD23	1:D:143:LEU:C	2.40	0.41
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.03	0.41
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.75	0.41
1:F:78:GLU:HG2	2:R:301:PRO:HB3	2.02	0.41
1:F:5:LEU:O	2:R:387:GLN:HG2	2.19	0.41
1:F:35:ILE:HD13	2:R:351:PHE:CE1	2.56	0.41
2:R:420:ASP:HA	2:R:421:PRO:HD2	1.78	0.41
1:D:58:GLY:HA3	1:D:190:GLN:OE1	2.21	0.41
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.67	0.41
2:M:403:ASN:HB2	6:M:610:HOH:O	2.21	0.41
2:Q:395:THR:O	2:Q:430:LEU:HA	2.21	0.41
1:A:54:GLN:HG2	1:A:102:GLY:O	2.21	0.41
1:D:67:PHE:HZ	1:D:94:ARG:CD	2.27	0.41
2:R:360:ASP:HB3	2:R:428:ARG:HG3	2.02	0.41
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.50	0.41
2:M:363:LEU:HD12	2:M:363:LEU:N	2.35	0.41
1:D:155:CYS:HA	1:D:156:PRO:HD2	1.94	0.41
1:A:176:GLU:HG3	1:A:180:LYS:N	2.35	0.41
2:R:414:ARG:N	2:R:414:ARG:HD2	2.36	0.41
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.21	0.41
1:C:110:LYS:NZ	1:C:147:ASP:OD1	2.52	0.41
1:E:158:LEU:HD12	1:E:158:LEU:HA	1.97	0.41
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:VAL:HA	1:F:127:ASN:O	2.22	0.40
2:O:331:SER:HA	2:O:332:PRO:HD3	1.96	0.40
2:Q:386:ASP:HA	2:Q:527:LEU:O	2.21	0.40
1:B:176:GLU:HA	1:B:180:LYS:O	2.20	0.40
1:B:52:LEU:HA	1:B:104:TRP:O	2.21	0.40
1:E:58:GLY:HA3	1:E:190:GLN:OE1	2.21	0.40
2:P:359:HIS:O	2:P:366:ASN:HB3	2.21	0.40
2:R:316:HIS:HB3	2:R:317:PRO:HD2	2.02	0.40
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.81	0.40
1:E:67:PHE:HZ	1:E:94:ARG:CD	2.25	0.40
1:F:66:SER:HA	1:F:132:ALA:HB2	2.04	0.40
2:P:390:LYS:HE2	6:P:720:HOH:O	2.21	0.40
1:B:73:ALA:HB1	1:B:78:GLU:N	2.37	0.40
2:O:390:LYS:CE	6:O:725:HOH:O	2.70	0.40
2:M:376:GLU:HG2	2:P:446:PRO:HD2	2.03	0.40
2:R:372:LEU:HA	2:R:373:PRO:HD3	2.00	0.40
2:R:304:ASP:HB2	2:R:343:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	D	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	E	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	F	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
2	M	229/238 (96%)	219 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
All	All	2562/2628 (98%)	2468 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	156 (96%)	6 (4%)	41	62
1	B	162/163 (99%)	155 (96%)	7 (4%)	35	55
1	C	162/163 (99%)	154 (95%)	8 (5%)	31	48
1	D	162/163 (99%)	156 (96%)	6 (4%)	41	62
1	E	162/163 (99%)	156 (96%)	6 (4%)	41	62
1	F	162/163 (99%)	156 (96%)	6 (4%)	41	62
2	M	196/202 (97%)	187 (95%)	9 (5%)	33	51
2	N	196/202 (97%)	189 (96%)	7 (4%)	42	63
2	O	196/202 (97%)	190 (97%)	6 (3%)	47	69
2	P	196/202 (97%)	185 (94%)	11 (6%)	26	41
2	Q	196/202 (97%)	188 (96%)	8 (4%)	37	57
2	R	196/202 (97%)	188 (96%)	8 (4%)	37	57
All	All	2148/2190 (98%)	2060 (96%)	88 (4%)	37	57

All (88) 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
1	A	52	LEU
1	A	106	LEU
1	A	165	GLN
2	M	395	THR
2	M	414	ARG
2	M	416	LEU
2	M	428	ARG
2	M	433	SER
2	M	434	ASP
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	158	LEU
1	B	165	GLN
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	428	ARG
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	94	ARG
1	C	133	ARG
1	C	165	GLN
1	C	181	THR
2	O	393	PRO
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	497	ASN
2	O	534	HIS

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Mol	Chain	Res	Type
1	D	19	ILE
1	D	38	ARG
1	D	43	ASP
1	D	52	LEU
1	D	154	LYS
1	D	165	GLN
2	P	364	LEU
2	P	395	THR
2	P	399	MET
2	P	416	LEU
2	P	428	ARG
2	P	434	ASP
2	P	440	ARG
2	P	478	LEU
2	P	497	ASN
2	P	499	GLU
2	P	534	HIS
1	E	19	ILE
1	E	32	ASP
1	E	52	LEU
1	E	94	ARG
1	E	165	GLN
1	E	188	ARG
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	478	LEU
2	Q	497	ASN
2	Q	507	LYS
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	66	SER
1	F	94	ARG
1	F	165	GLN
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP

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Mol	Chain	Res	Type
2	R	442	ILE
2	R	497	ASN
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	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
2	P	503	GLN
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	497	ASN
2	R	503	GLN
2	R	530	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	DHY	M	550[A]	3	9,12,12	1.30	2 (22%)	13,16,16	1.65	2 (15%)
5	DHY	M	550[B]	3	9,12,12	1.23	2 (22%)	13,16,16	1.71	4 (30%)
4	BME	M	601	2	3,3,3	0.32	0	2,2,2	0.60	0
5	DHY	N	550[A]	3	9,12,12	1.18	1 (11%)	13,16,16	1.75	3 (23%)
5	DHY	N	550[B]	3	9,12,12	1.22	1 (11%)	13,16,16	1.93	5 (38%)
4	BME	N	601	2	3,3,3	0.22	0	2,2,2	0.15	0
5	DHY	O	550[A]	3	9,12,12	1.42	1 (11%)	13,16,16	1.53	3 (23%)
5	DHY	O	550[B]	3	9,12,12	1.40	2 (22%)	13,16,16	1.86	4 (30%)
4	BME	O	601	2	3,3,3	0.47	0	2,2,2	0.37	0
5	DHY	P	550[A]	3	9,12,12	1.17	0	13,16,16	1.40	2 (15%)
5	DHY	P	550[B]	3	9,12,12	1.27	1 (11%)	13,16,16	1.69	4 (30%)
4	BME	P	601	2	3,3,3	0.54	0	2,2,2	0.94	0
5	DHY	Q	550[A]	3	9,12,12	1.18	1 (11%)	13,16,16	1.28	2 (15%)
5	DHY	Q	550[B]	3	9,12,12	1.19	1 (11%)	13,16,16	1.58	3 (23%)
4	BME	Q	601	2	3,3,3	0.50	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DHY	R	550[A]	3	9,12,12	1.42	2 (22%)	13,16,16	1.58	2 (15%)
5	DHY	R	550[B]	3	9,12,12	1.28	1 (11%)	13,16,16	1.65	4 (30%)
4	BME	R	601	2	3,3,3	0.33	0	2,2,2	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DHY	M	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	M	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	M	601	2	-	0/1/1/1	0/0/0/0
5	DHY	N	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	N	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	0/0/0/0
5	DHY	O	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	O	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	0/0/0/0
5	DHY	P	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	P	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	0/0/0/0
5	DHY	Q	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	Q	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	0/0/0/0
5	DHY	R	550[A]	3	-	0/2/4/4	0/1/1/1
5	DHY	R	550[B]	3	-	0/2/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	550[A]	DHY	C2-C1	2.04	1.42	1.39
5	M	550[A]	DHY	C6-C5	2.05	1.42	1.38
5	M	550[B]	DHY	C6-C5	2.11	1.42	1.38
5	N	550[A]	DHY	C2-C1	2.16	1.43	1.39
5	P	550[B]	DHY	C6-C1	2.29	1.43	1.38
5	R	550[A]	DHY	C6-C5	2.33	1.42	1.38
5	M	550[A]	DHY	C2-C1	2.45	1.43	1.39
5	O	550[B]	DHY	C6-C5	2.45	1.43	1.38
5	N	550[B]	DHY	C6-C1	2.46	1.44	1.38
5	R	550[A]	DHY	C2-C1	2.51	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	550[B]	DHY	C6-C1	2.54	1.44	1.38
5	M	550[B]	DHY	C6-C1	2.54	1.44	1.38
5	Q	550[B]	DHY	C6-C1	2.62	1.44	1.38
5	R	550[B]	DHY	C6-C1	2.77	1.44	1.38
5	O	550[A]	DHY	C2-C1	2.87	1.44	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	550[B]	DHY	C6-C5-C4	-3.62	116.77	120.49
5	O	550[B]	DHY	C6-C5-C4	-3.26	117.14	120.49
5	M	550[B]	DHY	C6-C5-C4	-3.13	117.28	120.49
5	N	550[A]	DHY	C3-C2-C1	-3.10	117.07	120.83
5	M	550[A]	DHY	C3-C2-C1	-2.89	117.33	120.83
5	P	550[B]	DHY	C6-C5-C4	-2.79	117.63	120.49
5	R	550[B]	DHY	C6-C5-C4	-2.66	117.77	120.49
5	O	550[A]	DHY	C3-C2-C1	-2.56	117.73	120.83
5	R	550[A]	DHY	C3-C2-C1	-2.44	117.87	120.83
5	Q	550[B]	DHY	C6-C5-C4	-2.44	117.99	120.49
5	Q	550[B]	DHY	C7-C1-C6	-2.37	113.66	120.90
5	N	550[B]	DHY	C7-C1-C6	-2.30	113.88	120.90
5	P	550[A]	DHY	C3-C2-C1	-2.29	118.06	120.83
5	M	550[B]	DHY	C7-C1-C6	-2.17	114.26	120.90
5	Q	550[A]	DHY	C3-C2-C1	-2.15	118.22	120.83
5	O	550[B]	DHY	C7-C1-C6	-2.13	114.39	120.90
5	R	550[B]	DHY	C7-C1-C6	-2.12	114.42	120.90
5	P	550[B]	DHY	C7-C1-C6	-2.11	114.43	120.90
5	N	550[A]	DHY	O4-C4-C5	2.02	124.89	119.35
5	O	550[A]	DHY	O4-C4-C5	2.02	124.91	119.35
5	O	550[B]	DHY	O3-C3-C2	2.03	124.89	119.42
5	Q	550[A]	DHY	C2-C3-C4	2.15	121.77	119.82
5	P	550[B]	DHY	C5-C4-C3	2.17	122.48	119.72
5	M	550[B]	DHY	C7-C1-C2	2.18	125.21	120.69
5	P	550[B]	DHY	C7-C1-C2	2.19	125.22	120.69
5	N	550[B]	DHY	C7-C1-C2	2.24	125.31	120.69
5	N	550[B]	DHY	O3-C3-C2	2.24	125.45	119.42
5	R	550[B]	DHY	C7-C1-C2	2.28	125.40	120.69
5	O	550[A]	DHY	C2-C3-C4	2.29	121.89	119.82
5	N	550[B]	DHY	C5-C4-C3	2.39	122.75	119.72
5	P	550[A]	DHY	C2-C3-C4	2.43	122.03	119.82
5	N	550[A]	DHY	C2-C3-C4	2.48	122.07	119.82
5	Q	550[B]	DHY	C7-C1-C2	2.54	125.95	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	550[B]	DHY	C5-C4-C3	2.62	123.05	119.72
5	O	550[B]	DHY	C5-C4-C3	2.67	123.11	119.72
5	M	550[B]	DHY	C5-C4-C3	2.79	123.27	119.72
5	R	550[A]	DHY	C2-C3-C4	2.86	122.42	119.82
5	M	550[A]	DHY	C2-C3-C4	2.97	122.51	119.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	550[A]	DHY	4	0
5	M	550[B]	DHY	4	0
4	M	601	BME	1	0
5	N	550[A]	DHY	5	0
5	N	550[B]	DHY	5	0
5	O	550[A]	DHY	4	0
5	O	550[B]	DHY	3	0
4	O	601	BME	1	0
5	P	550[A]	DHY	5	0
5	P	550[B]	DHY	3	0
5	Q	550[A]	DHY	6	0
5	Q	550[B]	DHY	5	0
4	Q	601	BME	3	0
5	R	550[A]	DHY	4	0
5	R	550[B]	DHY	4	0
4	R	601	BME	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.