



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:32 pm BST

PDB ID : 3PCG
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH THE INHIBITOR 4-HYDROXYPHENYLACETATE
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-04-29
Resolution : 1.96 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

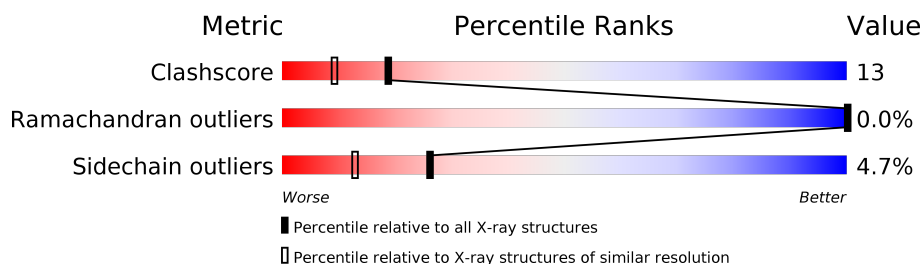
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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	68% 29% .
1	B	200	76% 21% ..
1	C	200	69% 28% ..
1	D	200	73% 23% ..
1	E	200	73% 23% ..
1	F	200	65% 31% ..
2	M	238	69% 25% ..
2	N	238	77% 18% ...

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	4HP	M	550	-	-	X	-
5	4HP	P	550	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21996 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			

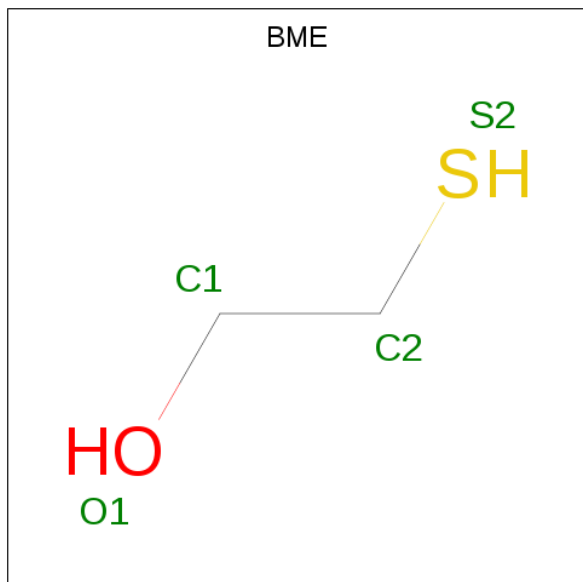
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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).

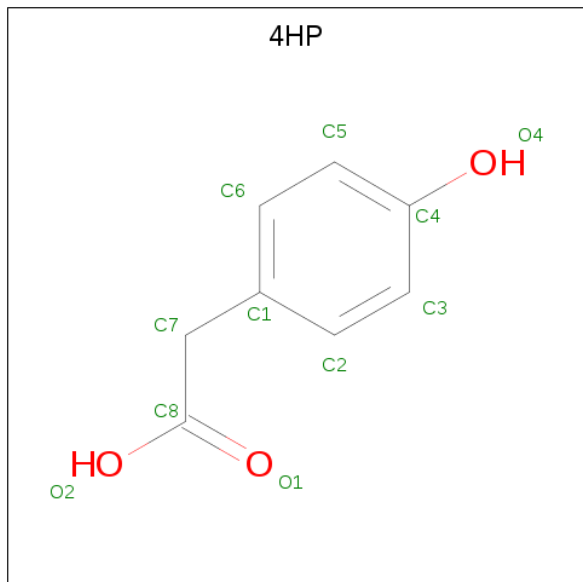
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- 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 4-HYDROXYPHENYLACETATE (three-letter code: 4HP) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	0
			11	8	3		
5	N	1	Total	C	O	0	0
			11	8	3		
5	O	1	Total	C	O	0	0
			11	8	3		
5	P	1	Total	C	O	0	0
			11	8	3		
5	Q	1	Total	C	O	0	0
			11	8	3		
5	R	1	Total	C	O	0	0
			11	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	M	161	Total	O	0	0
			161	161		
6	B	84	Total	O	0	0
			84	84		
6	N	161	Total	O	0	0
			161	161		

Continued on next page...

Continued from previous page...

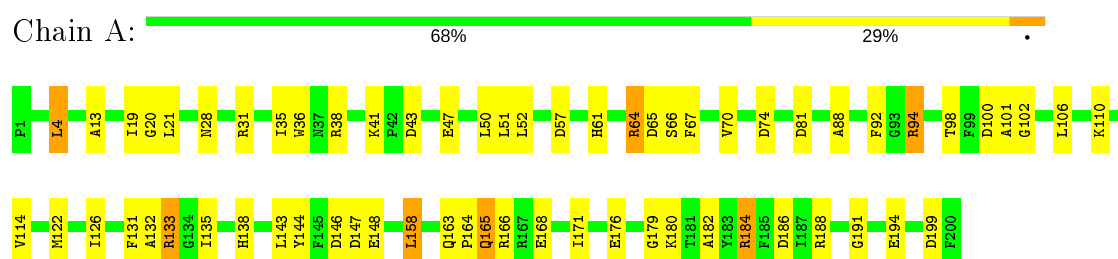
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	81	Total 81	O 81	0	0
6	O	157	Total 157	O 157	0	0
6	D	74	Total 74	O 74	0	0
6	P	158	Total 158	O 158	0	0
6	E	81	Total 81	O 81	0	0
6	Q	163	Total 163	O 163	0	0
6	F	78	Total 78	O 78	0	0
6	R	160	Total 160	O 160	0	0

3 Residue-property plots [i](#)

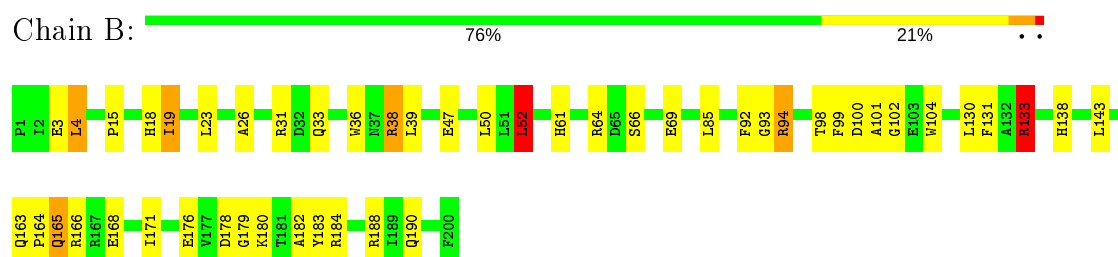
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

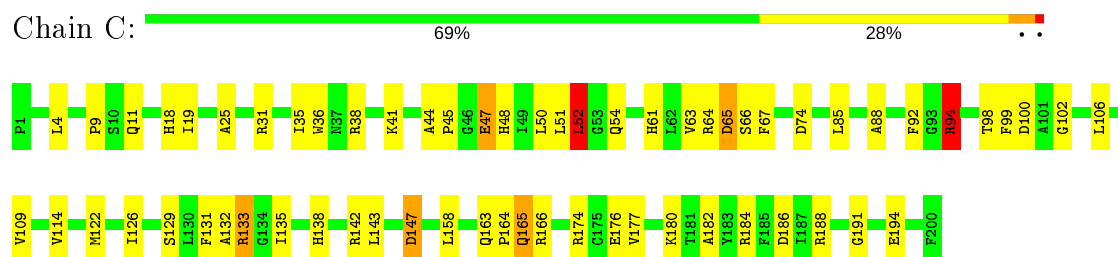
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



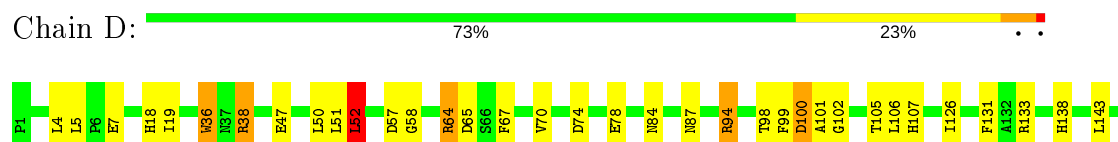
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE





• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E: 73% 23% . .



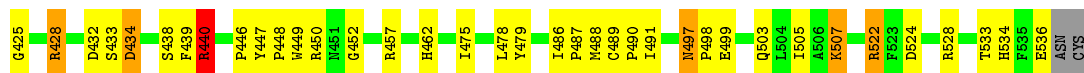
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F: 65% 31% . .



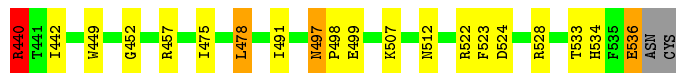
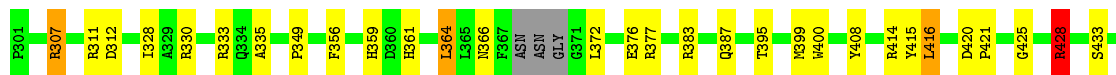
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M: 69% 25% . .



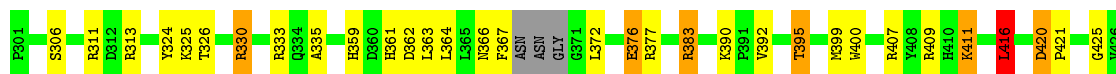
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

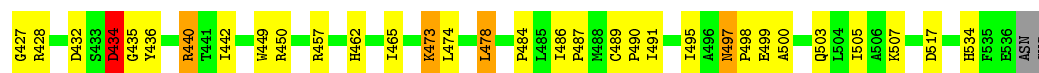
Chain N: 77% 18% . . .



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

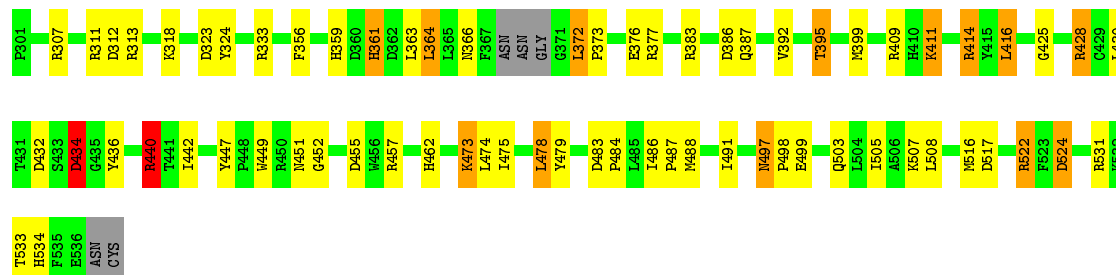
Chain O: 71% 22% . . .





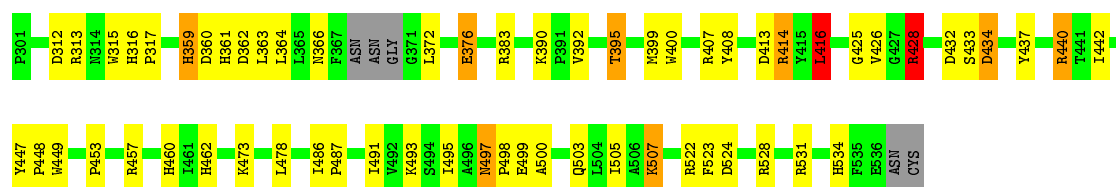
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 69% 22% 5% ..



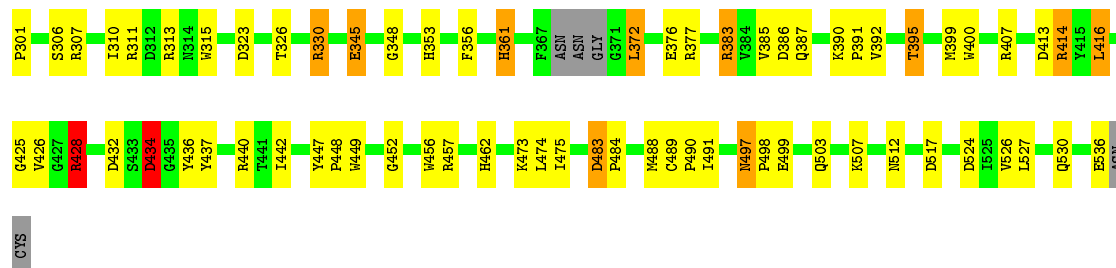
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 72% 21% ..



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 69% 24% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.32Å 127.12Å 134.13Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 1.96	Depositor
% Data completeness (in resolution range)	81.4 (6.00-1.96)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21996	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: BME, FE, 4HP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	3/1611 (0.2%)	1.88	32/2195 (1.5%)
1	B	0.98	0/1611	1.53	18/2195 (0.8%)
1	C	0.98	1/1611 (0.1%)	1.67	22/2195 (1.0%)
1	D	1.01	3/1611 (0.2%)	1.73	23/2195 (1.0%)
1	E	1.05	2/1611 (0.1%)	1.73	18/2195 (0.8%)
1	F	1.01	0/1611	1.55	20/2195 (0.9%)
2	M	1.11	2/1895 (0.1%)	1.67	32/2580 (1.2%)
2	N	1.07	1/1895 (0.1%)	1.59	20/2580 (0.8%)
2	O	1.07	0/1895	1.61	27/2580 (1.0%)
2	P	1.08	3/1895 (0.2%)	1.73	37/2580 (1.4%)
2	Q	1.10	2/1895 (0.1%)	1.66	27/2580 (1.0%)
2	R	1.08	1/1895 (0.1%)	1.67	31/2580 (1.2%)
All	All	1.05	18/21036 (0.1%)	1.67	307/28650 (1.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	94	ARG	CD-NE	-9.44	1.30	1.46
1	A	94	ARG	CD-NE	-8.80	1.31	1.46
2	M	428	ARG	CD-NE	-6.68	1.35	1.46
2	Q	440	ARG	CD-NE	-6.54	1.35	1.46
1	C	94	ARG	CD-NE	-6.34	1.35	1.46
1	A	66	SER	CB-OG	-6.28	1.34	1.42
2	P	428	ARG	CD-NE	-6.25	1.35	1.46
2	P	440	ARG	CD-NE	-6.24	1.35	1.46
2	R	428	ARG	CD-NE	-6.17	1.35	1.46
1	D	94	ARG	CD-NE	-6.11	1.36	1.46
1	D	7	GLU	CD-OE2	-5.89	1.19	1.25
2	P	428	ARG	CG-CD	-5.76	1.37	1.51
2	Q	433	SER	CB-OG	5.76	1.49	1.42
1	A	47	GLU	CB-CG	-5.70	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	440	ARG	CD-NE	-5.55	1.37	1.46
1	D	133	ARG	CD-NE	-5.46	1.37	1.46
2	M	452	GLY	CA-C	5.27	1.60	1.51
1	E	47	GLU	CB-CG	-5.09	1.42	1.52

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	27.73	162.42	123.60
1	A	47	GLU	CA-CB-CG	27.09	172.99	113.40
1	D	133	ARG	CD-NE-CZ	26.11	160.16	123.60
2	N	440	ARG	NE-CZ-NH2	-22.36	109.12	120.30
2	M	440	ARG	NE-CZ-NH2	-22.30	109.15	120.30
2	P	440	ARG	NE-CZ-NH2	-22.25	109.17	120.30
2	Q	440	ARG	NE-CZ-NH2	-21.89	109.35	120.30
1	E	47	GLU	CA-CB-CG	21.53	160.76	113.40
2	O	440	ARG	NE-CZ-NH2	-21.44	109.58	120.30
1	E	94	ARG	CD-NE-CZ	21.30	153.42	123.60
1	E	94	ARG	NE-CZ-NH1	19.91	130.26	120.30
1	C	133	ARG	NE-CZ-NH1	18.92	129.76	120.30
1	C	94	ARG	CD-NE-CZ	18.74	149.84	123.60
2	R	440	ARG	NE-CZ-NH2	-18.74	110.93	120.30
1	D	94	ARG	NE-CZ-NH2	-18.17	111.22	120.30
1	C	94	ARG	NE-CZ-NH1	17.12	128.86	120.30
1	D	94	ARG	NE-CZ-NH1	16.80	128.70	120.30
2	P	428	ARG	NE-CZ-NH1	15.81	128.21	120.30
2	Q	457	ARG	NE-CZ-NH1	15.49	128.05	120.30
1	C	94	ARG	NE-CZ-NH2	-14.86	112.87	120.30
2	P	428	ARG	NE-CZ-NH2	-14.57	113.01	120.30
1	A	166	ARG	NE-CZ-NH1	14.57	127.58	120.30
2	M	414	ARG	NE-CZ-NH1	14.20	127.40	120.30
2	R	428	ARG	NE-CZ-NH2	-14.06	113.27	120.30
1	E	94	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	E	94	ARG	CG-CD-NE	13.95	141.10	111.80
1	D	133	ARG	NE-CZ-NH1	13.75	127.17	120.30
2	R	428	ARG	CD-NE-CZ	13.70	142.78	123.60
1	A	94	ARG	NE-CZ-NH2	-13.63	113.49	120.30
2	R	428	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	A	94	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	A	184	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	A	94	ARG	CG-CD-NE	12.29	137.61	111.80
2	Q	428	ARG	NE-CZ-NH2	-12.14	114.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	440	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	D	166	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	F	47	GLU	CA-CB-CG	11.73	139.21	113.40
1	D	94	ARG	CD-NE-CZ	11.64	139.89	123.60
2	O	383	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	D	47	GLU	CA-CB-CG	11.51	138.73	113.40
2	P	428	ARG	CG-CD-NE	11.49	135.93	111.80
1	A	133	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	B	184	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	B	47	GLU	CA-CB-CG	11.20	138.05	113.40
2	R	307	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	M	428	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	C	133	ARG	CD-NE-CZ	11.05	139.07	123.60
2	P	428	ARG	CD-NE-CZ	10.99	138.99	123.60
1	F	94	ARG	NE-CZ-NH1	10.93	125.77	120.30
2	M	330	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	N	428	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	133	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	D	166	ARG	NE-CZ-NH1	10.77	125.69	120.30
2	Q	457	ARG	NE-CZ-NH2	-10.69	114.95	120.30
1	F	94	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	M	428	ARG	NE-CZ-NH2	-10.46	115.07	120.30
2	P	440	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	M	428	ARG	CG-CD-NE	10.13	133.06	111.80
2	M	428	ARG	CD-NE-CZ	10.12	137.78	123.60
2	R	457	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	A	166	ARG	NE-CZ-NH2	-9.88	115.36	120.30
2	P	428	ARG	CB-CG-CD	9.62	136.61	111.60
2	M	528	ARG	NE-CZ-NH2	-9.52	115.54	120.30
2	M	414	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	A	188	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	31	ARG	NE-CZ-NH2	-9.28	115.66	120.30
2	P	383	ARG	NE-CZ-NH1	-9.17	115.72	120.30
2	R	330	ARG	NE-CZ-NH1	9.17	124.88	120.30
2	N	428	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	A	31	ARG	NE-CZ-NH1	9.10	124.85	120.30
2	O	333	ARG	NE-CZ-NH2	-9.09	115.75	120.30
2	O	313	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	188	ARG	NE-CZ-NH1	8.85	124.72	120.30
2	R	440	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	P	386	ASP	CB-CG-OD2	8.68	126.11	118.30
2	P	524	ASP	CB-CG-OD2	-8.67	110.50	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	457	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	E	31	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	C	166	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	M	440	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	C	142	ARG	NE-CZ-NH2	-8.33	116.13	120.30
2	M	522	ARG	NE-CZ-NH2	8.33	124.46	120.30
2	Q	440	ARG	CD-NE-CZ	8.29	135.21	123.60
2	O	428	ARG	CD-NE-CZ	8.26	135.17	123.60
2	R	428	ARG	CG-CD-NE	8.26	129.14	111.80
1	E	31	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	P	440	ARG	CD-NE-CZ	8.25	135.15	123.60
2	R	434	ASP	CB-CG-OD2	-8.23	110.89	118.30
2	M	312	ASP	CB-CG-OD1	8.21	125.69	118.30
2	O	432	ASP	CB-CG-OD1	8.18	125.66	118.30
2	P	522	ARG	NE-CZ-NH1	-8.11	116.24	120.30
2	O	330	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	B	188	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	F	142	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	E	133	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	C	133	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	E	74	ASP	CB-CG-OD1	7.92	125.42	118.30
2	P	457	ARG	CD-NE-CZ	7.89	134.65	123.60
1	A	184	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	65	ASP	CB-CG-OD1	7.88	125.39	118.30
1	C	47	GLU	CA-CB-CG	7.87	130.70	113.40
2	R	457	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	M	383	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	E	38	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	D	188	ARG	NE-CZ-NH1	7.81	124.21	120.30
2	N	457	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	R	432	ASP	CB-CG-OD2	-7.80	111.28	118.30
2	Q	432	ASP	CB-CG-OD1	7.71	125.24	118.30
2	Q	522	ARG	NE-CZ-NH1	-7.69	116.46	120.30
2	N	312	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	65	ASP	CB-CG-OD1	7.64	125.17	118.30
1	A	64	ARG	NE-CZ-NH1	-7.63	116.48	120.30
2	N	457	ARG	NE-CZ-NH2	-7.60	116.50	120.30
2	P	333	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	D	184	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	O	440	ARG	NH1-CZ-NH2	7.39	127.53	119.40
2	M	450	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	F	166	ARG	NE-CZ-NH1	7.31	123.95	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	432	ASP	CB-CG-OD2	-7.31	111.72	118.30
2	R	524	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	57	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	166	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	N	428	ARG	CG-CD-NE	7.21	126.93	111.80
1	D	188	ARG	NE-CZ-NH2	-7.19	116.70	120.30
2	N	440	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	B	166	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	B	188	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	57	ASP	CB-CG-OD2	-7.06	111.95	118.30
2	Q	457	ARG	CD-NE-CZ	7.02	133.43	123.60
2	P	479	TYR	CB-CG-CD1	-7.01	116.80	121.00
2	Q	428	ARG	NE-CZ-NH1	6.97	123.79	120.30
2	Q	524	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	M	434	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	E	65	ASP	CB-CG-OD1	6.95	124.56	118.30
2	M	414	ARG	CD-NE-CZ	6.93	133.30	123.60
2	M	323	ASP	CB-CG-OD2	-6.89	112.10	118.30
2	N	440	ARG	NH1-CZ-NH2	6.87	126.96	119.40
1	D	74	ASP	CB-CG-OD1	6.83	124.45	118.30
1	E	166	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	94	ARG	CB-CG-CD	6.77	129.21	111.60
1	D	64	ARG	NE-CZ-NH2	-6.77	116.91	120.30
2	Q	531	ARG	NE-CZ-NH1	6.75	123.68	120.30
2	O	376	GLU	OE1-CD-OE2	6.72	131.37	123.30
1	F	43	ASP	CB-CG-OD1	-6.72	112.25	118.30
2	P	434	ASP	CB-CG-OD1	-6.71	112.26	118.30
2	P	522	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	B	94	ARG	CD-NE-CZ	6.67	132.94	123.60
2	M	432	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	133	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	O	311	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	D	94	ARG	CG-CD-NE	6.63	125.72	111.80
2	R	414	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	O	409	ARG	CD-NE-CZ	-6.61	114.35	123.60
1	F	188	ARG	NE-CZ-NH1	6.59	123.59	120.30
2	R	483	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	E	52	LEU	CB-CA-C	6.52	122.58	110.20
1	B	178	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	147	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	M	450	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	N	383	ARG	NE-CZ-NH2	-6.43	117.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	NE-CZ-NH1	6.43	123.51	120.30
2	N	524	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	Q	376	GLU	OE1-CD-OE2	6.37	130.95	123.30
2	O	407	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	N	522	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	38	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	R	377	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	N	311	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	Q	407	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	R	383	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	N	330	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	Q	531	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	F	36	TRP	CB-CA-C	6.08	122.55	110.40
2	N	428	ARG	CB-CG-CD	6.04	127.31	111.60
2	O	409	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	F	162	GLU	CA-CB-CG	6.03	126.67	113.40
2	P	414	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	158	LEU	CB-CA-C	6.02	121.64	110.20
1	A	66	SER	CB-CA-C	-5.99	98.72	110.10
2	M	457	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	N	307	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	O	377	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	R	330	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	Q	416	LEU	CB-CA-C	5.92	121.45	110.20
1	F	106	LEU	CA-CB-CG	5.92	128.91	115.30
2	P	524	ASP	CB-CG-OD1	5.91	123.62	118.30
1	E	133	ARG	CD-NE-CZ	5.91	131.87	123.60
2	P	432	ASP	CB-CG-OD1	5.90	123.61	118.30
2	M	522	ARG	NE-CZ-NH1	-5.90	117.35	120.30
2	Q	434	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	M	323	ASP	CB-CG-OD1	5.89	123.60	118.30
1	E	36	TRP	CB-CA-C	5.89	122.17	110.40
1	A	64	ARG	CD-NE-CZ	-5.88	115.36	123.60
2	P	377	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	B	133	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	P	457	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	52	LEU	CB-CA-C	5.86	121.33	110.20
2	Q	528	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	M	440	ARG	NH1-CZ-NH2	5.84	125.82	119.40
2	Q	312	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	57	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	65	ASP	CB-CG-OD1	5.79	123.51	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	434	ASP	OD1-CG-OD2	5.79	134.31	123.30
1	A	186	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	188	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	P	531	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	N	536	GLU	CG-CD-OE1	5.76	129.83	118.30
1	C	31	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	N	377	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	129	SER	N-CA-CB	5.74	119.10	110.50
2	N	528	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	183	TYR	N-CA-CB	5.72	120.90	110.60
2	Q	313	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	36	TRP	CB-CA-C	5.69	121.78	110.40
1	C	52	LEU	CB-CA-C	5.69	121.01	110.20
1	C	65	ASP	CB-CG-OD2	-5.69	113.18	118.30
2	R	432	ASP	CB-CG-OD1	5.68	123.42	118.30
2	M	312	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	186	ASP	CB-CG-OD2	-5.65	113.22	118.30
2	R	414	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	Q	414	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	R	323	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	P	372	LEU	CB-CA-C	5.64	120.91	110.20
1	F	100	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	36	TRP	CB-CA-C	5.63	121.66	110.40
1	D	133	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	O	416	LEU	CB-CA-C	5.58	120.80	110.20
2	M	457	ARG	CD-NE-CZ	5.56	131.39	123.60
1	C	74	ASP	CB-CG-OD1	5.56	123.30	118.30
1	F	52	LEU	CB-CA-C	5.55	120.75	110.20
2	R	452	GLY	N-CA-C	-5.54	99.25	113.10
2	P	312	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	Q	428	ARG	CD-NE-CZ	5.52	131.33	123.60
2	O	313	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	R	361	HIS	CA-CB-CG	-5.51	104.23	113.60
1	C	36	TRP	CB-CA-C	5.50	121.41	110.40
2	Q	437	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	E	166	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	147	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	F	141	THR	CA-CB-CG2	5.47	120.06	112.40
2	M	479	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	F	65	ASP	CB-CG-OD1	5.45	123.21	118.30
2	P	323	ASP	CB-CG-OD1	5.44	123.19	118.30
2	O	517	ASP	CB-CG-OD2	-5.43	113.41	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	311	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	11	GLN	N-CA-CB	5.41	120.33	110.60
1	A	147	ASP	CB-CG-OD1	5.39	123.15	118.30
1	F	184	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	C	25	ALA	CB-CA-C	5.39	118.18	110.10
2	O	450	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	R	345	GLU	OE1-CD-OE2	5.36	129.73	123.30
2	P	333	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	B	52	LEU	CA-CB-CG	5.34	127.59	115.30
2	N	452	GLY	N-CA-C	-5.33	99.78	113.10
2	P	473	LYS	CA-CB-CG	5.31	125.08	113.40
1	D	174	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	O	434	ASP	CA-CB-CG	-5.30	101.75	113.40
2	M	432	ASP	CB-CG-OD1	5.27	123.05	118.30
2	O	407	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	O	434	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	F	158	LEU	CB-CA-C	5.26	120.20	110.20
2	P	440	ARG	NH1-CZ-NH2	5.25	125.18	119.40
1	F	162	GLU	N-CA-CB	5.25	120.05	110.60
2	O	383	ARG	NH1-CZ-NH2	5.25	125.17	119.40
2	Q	383	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	O	377	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	F	38	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	R	353	HIS	CA-CB-CG	-5.24	104.69	113.60
2	M	528	ARG	NH1-CZ-NH2	5.24	125.16	119.40
1	D	36	TRP	CB-CA-C	5.23	120.86	110.40
2	Q	440	ARG	CB-CG-CD	-5.23	98.00	111.60
2	P	517	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	178	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	F	47	GLU	N-CA-CB	5.21	119.97	110.60
2	P	311	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	M	522	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	A	158	LEU	CB-CA-C	5.19	120.07	110.20
2	O	440	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	R	407	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	R	323	ASP	CB-CG-OD1	5.18	122.96	118.30
2	P	447	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	81	ASP	CB-CG-OD2	-5.17	113.64	118.30
2	M	452	GLY	N-CA-C	-5.16	100.19	113.10
1	A	74	ASP	CB-CG-OD1	5.15	122.93	118.30
1	D	186	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	31	ARG	CD-NE-CZ	5.15	130.80	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	LEU	CB-CA-C	5.14	119.97	110.20
1	C	158	LEU	CB-CA-C	5.14	119.96	110.20
2	P	452	GLY	N-CA-C	-5.13	100.27	113.10
1	A	31	ARG	CD-NE-CZ	5.12	130.78	123.60
2	R	313	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	D	184	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	186	ASP	CB-CG-OD2	-5.12	113.70	118.30
2	P	409	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	P	361	HIS	CA-CB-CG	-5.11	104.91	113.60
2	M	439	PHE	O-C-N	5.09	130.84	122.70
1	F	183	TYR	CA-CB-CG	5.08	123.06	113.40
2	O	367	PHE	CA-C-O	-5.07	109.46	120.10
2	O	420	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	13	ALA	CB-CA-C	5.06	117.69	110.10
1	A	146	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	M	428	ARG	CB-CG-CD	5.05	124.74	111.60
2	R	517	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	D	78	GLU	OE1-CD-OE2	5.03	129.34	123.30
2	Q	359	HIS	CA-CB-CG	-5.03	105.05	113.60
2	P	483	ASP	CB-CG-OD2	5.01	122.81	118.30
2	P	414	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	44	0
1	B	1571	0	1499	47	0
1	C	1571	0	1499	47	0
1	D	1571	0	1499	39	0
1	E	1571	0	1499	47	0
1	F	1571	0	1499	67	0
2	M	1840	0	1792	55	0
2	N	1840	0	1792	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1840	0	1792	47	0
2	P	1840	0	1792	46	0
2	Q	1840	0	1792	44	0
2	R	1840	0	1792	53	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	3	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	1	0
4	R	4	0	5	0	0
5	M	11	0	6	4	0
5	N	11	0	6	2	0
5	O	11	0	6	3	0
5	P	11	0	6	5	0
5	Q	11	0	6	2	0
5	R	11	0	6	3	0
6	A	76	0	0	2	0
6	B	84	0	0	1	0
6	C	81	0	0	1	0
6	D	74	0	0	2	0
6	E	81	0	0	1	0
6	F	78	0	0	3	0
6	M	161	0	0	2	0
6	N	161	0	0	1	0
6	O	157	0	0	2	0
6	P	158	0	0	1	0
6	Q	163	0	0	3	0
6	R	160	0	0	4	0
All	All	21996	0	19812	529	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 13.

All (529) 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:D:165:GLN:NE2	1:D:165:GLN:H	1.29	1.30
1:D:165:GLN:N	1:D:165:GLN:HE21	1.42	1.15
1:E:165:GLN:NE2	1:E:165:GLN:H	1.45	1.12
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.05	1.10
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.35	1.08
1:E:165:GLN:N	1:E:165:GLN:HE21	1.49	1.07
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.69	1.07
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.19	1.01
1:A:98:THR:HB	1:A:100:ASP:OD1	1.58	1.01
1:C:64:ARG:NH1	1:C:100:ASP:O	1.93	1.01
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.19	1.00
1:B:165:GLN:NE2	1:B:165:GLN:H	1.60	0.99
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.77	0.98
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.46	0.98
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.82	0.94
1:C:165:GLN:H	1:C:165:GLN:NE2	1.67	0.92
1:F:165:GLN:NE2	1:F:165:GLN:H	1.67	0.91
1:B:18:HIS:ND1	6:B:473:HOH:O	2.02	0.91
1:F:98:THR:HB	1:F:100:ASP:OD1	1.70	0.91
1:C:98:THR:OG1	1:C:102:GLY:N	2.05	0.90
1:D:98:THR:OG1	1:D:102:GLY:N	2.05	0.90
1:D:64:ARG:NH1	1:D:100:ASP:O	2.04	0.89
2:R:361:HIS:H	2:R:361:HIS:CD2	1.88	0.89
2:P:313:ARG:O	2:P:318:LYS:HE2	1.74	0.88
1:F:98:THR:OG1	1:F:102:GLY:N	2.06	0.88
2:M:390:LYS:HD2	6:M:644:HOH:O	1.74	0.88
1:B:165:GLN:CD	1:B:165:GLN:H	1.76	0.87
1:B:165:GLN:N	1:B:165:GLN:NE2	2.23	0.87
1:B:163:GLN:CB	1:B:165:GLN:HE22	1.89	0.85
1:F:180:LYS:HD2	1:F:181:THR:N	1.90	0.85
1:B:176:GLU:HG3	1:B:180:LYS:O	1.75	0.85
1:C:165:GLN:H	1:C:165:GLN:HE21	1.23	0.85
1:F:64:ARG:NH1	1:F:100:ASP:O	2.09	0.85
2:P:491:ILE:HD11	5:P:550:4HP:H71	1.57	0.85
2:R:361:HIS:H	2:R:361:HIS:HD2	1.24	0.85
1:A:98:THR:OG1	1:A:102:GLY:N	2.10	0.84
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.60	0.84
2:O:497:ASN:ND2	2:O:499:GLU:H	1.76	0.84
1:E:98:THR:OG1	1:E:102:GLY:N	2.11	0.83
1:D:98:THR:HB	1:D:100:ASP:OD1	1.77	0.83
2:O:390:LYS:HE2	6:O:729:HOH:O	1.77	0.83
2:O:497:ASN:HD22	2:O:499:GLU:H	1.25	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.07	0.82
1:F:163:GLN:CB	1:F:165:GLN:HE22	1.93	0.82
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.46	0.81
1:F:165:GLN:CD	1:F:165:GLN:H	1.82	0.81
1:C:18:HIS:ND1	6:C:281:HOH:O	2.08	0.81
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.80	0.81
2:M:361:HIS:H	2:M:361:HIS:CD2	1.98	0.81
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.64	0.80
2:P:411:LYS:O	2:P:414:ARG:NH1	2.14	0.80
1:E:98:THR:HB	1:E:100:ASP:OD1	1.82	0.80
2:N:497:ASN:HD22	2:N:499:GLU:H	1.31	0.79
2:Q:390:LYS:HD2	6:Q:1032:HOH:O	1.82	0.79
2:R:497:ASN:HD22	2:R:499:GLU:H	1.29	0.79
2:M:497:ASN:HD22	2:M:499:GLU:H	1.30	0.79
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	1.84	0.78
2:M:497:ASN:ND2	2:M:499:GLU:H	1.80	0.77
1:F:18:HIS:ND1	6:F:1429:HOH:O	2.17	0.77
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.84	0.77
1:A:163:GLN:CB	1:A:165:GLN:HE22	1.96	0.77
1:D:165:GLN:N	1:D:165:GLN:NE2	2.14	0.76
1:D:18:HIS:ND1	6:D:951:HOH:O	2.19	0.76
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.02	0.75
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.52	0.75
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.01	0.75
2:R:497:ASN:ND2	2:R:499:GLU:H	1.85	0.75
2:M:491:ILE:HD11	5:M:550:4HP:H71	1.68	0.75
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.67	0.75
1:E:64:ARG:NH1	1:E:100:ASP:O	2.20	0.74
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.23	0.73
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.70	0.73
1:A:165:GLN:H	1:A:165:GLN:CD	1.91	0.72
1:B:176:GLU:HG3	1:B:180:LYS:C	2.10	0.72
1:D:177:VAL:O	1:D:180:LYS:HB3	1.90	0.71
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.71	0.71
2:M:361:HIS:HD2	2:M:361:HIS:H	1.37	0.71
1:C:98:THR:HB	1:C:100:ASP:OD1	1.91	0.71
2:R:473:LYS:HD2	2:R:474:LEU:N	2.05	0.71
1:B:98:THR:HB	1:B:100:ASP:OD1	1.91	0.70
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.23	0.70
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.39	0.70
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.18	0.70
2:N:497:ASN:ND2	2:N:499:GLU:H	1.88	0.70
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.26	0.70
2:O:491:ILE:HD11	5:O:550:4HP:H71	1.74	0.70
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.57	0.69
1:F:64:ARG:HD3	1:F:99:PHE:O	1.92	0.69
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.11	0.69
1:D:165:GLN:HE21	1:D:165:GLN:H	0.72	0.69
2:M:449:TRP:CE3	5:M:550:4HP:H72	2.28	0.68
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.09	0.68
2:P:478:LEU:C	2:P:478:LEU:HD23	2.14	0.68
2:R:390:LYS:HD3	6:R:1271:HOH:O	1.95	0.68
1:A:64:ARG:NH1	1:A:100:ASP:O	2.27	0.67
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.75	0.67
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.77	0.67
2:Q:390:LYS:HD3	6:Q:1150:HOH:O	1.95	0.67
1:C:165:GLN:N	1:C:165:GLN:HE21	1.92	0.66
1:E:100:ASP:CG	1:E:101:ALA:H	1.99	0.66
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.30	0.66
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.94	0.66
2:O:449:TRP:CE3	5:O:550:4HP:H72	2.31	0.66
1:A:176:GLU:HG3	1:A:180:LYS:O	1.97	0.65
1:F:180:LYS:HD2	1:F:181:THR:H	1.60	0.65
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.62	0.64
1:F:77:GLY:O	1:F:114:VAL:HG12	1.97	0.64
2:P:491:ILE:CD1	5:P:550:4HP:H71	2.27	0.64
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.97	0.64
2:N:491:ILE:HD11	5:N:550:4HP:H71	1.79	0.64
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.12	0.64
2:P:361:HIS:CD2	2:P:361:HIS:H	2.16	0.64
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.80	0.64
2:R:536:GLU:HB2	6:R:1352:HOH:O	1.98	0.63
2:P:324:TYR:OH	5:P:550:4HP:O1	2.10	0.63
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.80	0.63
1:F:165:GLN:NE2	1:F:165:GLN:N	2.44	0.63
1:C:100:ASP:OD1	1:C:100:ASP:N	2.30	0.63
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.67	0.63
2:O:361:HIS:CD2	2:O:361:HIS:H	2.15	0.63
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.79	0.63
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.33	0.62
1:B:3:GLU:OE1	1:B:3:GLU:HA	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.81	0.62
1:F:98:THR:O	1:F:102:GLY:HA2	1.99	0.62
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.82	0.62
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.98	0.62
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.81	0.61
1:B:64:ARG:NH1	1:B:100:ASP:O	2.34	0.61
1:F:100:ASP:CG	1:F:101:ALA:H	2.03	0.61
1:F:48:HIS:C	1:F:180:LYS:NZ	2.54	0.61
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.15	0.61
2:O:399:MET:HA	2:O:462:HIS:O	2.00	0.61
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.46	0.61
2:R:390:LYS:HE2	6:R:1389:HOH:O	1.99	0.61
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.83	0.61
2:R:434:ASP:HB3	2:R:436:TYR:CD2	2.35	0.60
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.63	0.60
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.01	0.60
1:D:176:GLU:HA	1:D:180:LYS:O	2.01	0.60
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.37	0.60
2:N:449:TRP:CE3	5:N:550:4HP:H72	2.37	0.60
1:B:176:GLU:HA	1:B:180:LYS:O	2.02	0.60
1:F:48:HIS:C	1:F:180:LYS:HZ2	2.05	0.59
2:Q:449:TRP:CE3	5:Q:550:4HP:H72	2.37	0.59
2:R:491:ILE:HD11	5:R:550:4HP:H71	1.84	0.59
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.67	0.59
2:N:478:LEU:C	2:N:478:LEU:HD23	2.22	0.59
1:F:115:ASN:HA	1:F:121:PRO:HA	1.83	0.59
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.49	0.59
1:A:100:ASP:CG	1:A:101:ALA:H	2.04	0.59
1:B:52:LEU:HA	1:B:104:TRP:O	2.03	0.59
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.17	0.59
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.37	0.59
1:D:180:LYS:HG3	1:D:181:THR:N	2.18	0.59
1:D:64:ARG:HD3	1:D:99:PHE:O	2.04	0.58
1:C:99:PHE:HE2	2:O:411:LYS:HD2	1.68	0.58
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.03	0.58
1:E:61:HIS:CE1	1:F:163:GLN:HG3	2.38	0.58
1:F:35:ILE:HG21	1:F:92:PHE:HE2	1.67	0.58
1:C:177:VAL:O	1:C:180:LYS:HB3	2.04	0.58
2:R:361:HIS:N	2:R:361:HIS:CD2	2.60	0.57
2:R:400:TRP:HA	2:R:425:GLY:O	2.03	0.57
1:B:165:GLN:CA	1:B:165:GLN:HE21	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:PHE:CG	2:N:349:PRO:HG3	2.40	0.57
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.84	0.57
1:F:155:CYS:O	1:F:159:ASN:ND2	2.34	0.57
1:F:50:LEU:O	1:F:182:ALA:HA	2.04	0.57
2:R:497:ASN:HD22	2:R:497:ASN:C	2.08	0.57
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.19	0.57
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.08	0.56
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.35	0.56
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.39	0.56
2:P:364:LEU:HD12	2:P:373:PRO:HG2	1.88	0.56
1:F:70:VAL:HG11	1:F:106:LEU:HD21	1.88	0.56
2:M:413:ASP:C	2:M:414:ARG:HD2	2.26	0.56
1:A:70:VAL:HG21	1:A:106:LEU:HD21	1.86	0.56
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.36	0.56
2:M:478:LEU:C	2:M:478:LEU:HD23	2.26	0.56
2:N:416:LEU:C	2:N:416:LEU:HD23	2.25	0.56
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.40	0.56
1:C:48:HIS:HA	1:C:109:VAL:HG12	1.87	0.55
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.06	0.55
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.88	0.55
2:M:497:ASN:HD22	2:M:499:GLU:N	2.03	0.55
2:Q:316:HIS:HB3	2:Q:317:PRO:HD2	1.88	0.55
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.89	0.55
2:O:361:HIS:CG	4:O:601:BME:H21	2.41	0.55
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.87	0.55
2:M:497:ASN:HD22	2:M:497:ASN:C	2.10	0.55
2:P:462:HIS:HE1	5:P:550:4HP:H3	1.71	0.55
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.88	0.55
2:P:473:LYS:HD2	2:P:474:LEU:N	2.21	0.55
1:B:165:GLN:N	1:B:165:GLN:HE21	2.01	0.55
1:F:131:PHE:O	1:F:132:ALA:HB2	2.07	0.55
2:O:434:ASP:HB3	2:O:436:TYR:CE2	2.42	0.55
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.42	0.54
1:B:176:GLU:HG2	1:B:179:GLY:CA	2.37	0.54
1:F:49:ILE:HA	1:F:180:LYS:HE3	1.89	0.54
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.42	0.54
2:N:414:ARG:NE	2:N:414:ARG:HA	2.22	0.54
2:O:497:ASN:HD22	2:O:497:ASN:C	2.10	0.54
2:Q:413:ASP:C	2:Q:414:ARG:HD2	2.27	0.54
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.89	0.54
2:R:473:LYS:HD2	2:R:474:LEU:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HA	1:A:180:LYS:O	2.08	0.54
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.23	0.54
1:F:54:GLN:HG3	1:F:184:ARG:NH2	2.23	0.53
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.54	0.53
2:N:359:HIS:O	2:N:366:ASN:HB3	2.09	0.53
1:A:20:GLY:O	1:A:21:LEU:HD23	2.08	0.53
2:O:465:ILE:N	2:O:465:ILE:HD12	2.23	0.53
1:E:98:THR:HG1	1:E:103:GLU:H	1.57	0.53
2:N:497:ASN:HD22	2:N:499:GLU:N	2.03	0.53
2:P:361:HIS:HD2	2:P:361:HIS:H	1.57	0.53
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.73	0.53
2:M:505:ILE:O	2:M:507:LYS:HE3	2.08	0.53
1:F:180:LYS:HE3	1:F:181:THR:O	2.08	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.09	0.53
1:D:98:THR:O	1:D:102:GLY:HA2	2.09	0.52
1:F:35:ILE:HG21	1:F:92:PHE:CE2	2.43	0.52
1:F:18:HIS:CG	6:F:1429:HOH:O	2.59	0.52
2:P:497:ASN:ND2	2:P:499:GLU:H	2.07	0.52
2:R:434:ASP:HB3	2:R:436:TYR:CE2	2.45	0.52
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.44	0.52
2:M:414:ARG:HD2	2:M:414:ARG:N	2.23	0.52
1:E:98:THR:O	1:E:102:GLY:HA2	2.10	0.52
2:M:536:GLU:HB2	6:M:699:HOH:O	2.10	0.52
1:C:147:ASP:OD2	1:C:174:ARG:NH1	2.41	0.52
1:D:38:ARG:HG3	1:D:107:HIS:HB2	1.92	0.52
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.52
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.25	0.51
1:E:176:GLU:HG3	1:E:180:LYS:O	2.10	0.51
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.45	0.51
1:F:100:ASP:N	1:F:100:ASP:OD1	2.35	0.51
2:M:497:ASN:HD22	2:M:498:PRO:N	2.07	0.51
1:D:100:ASP:CG	1:D:101:ALA:H	2.13	0.51
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.10	0.51
1:D:52:LEU:C	1:D:52:LEU:HD22	2.30	0.51
2:M:373:PRO:HB3	2:M:423:PHE:HB2	1.93	0.51
2:O:497:ASN:HD21	2:O:499:GLU:HB2	1.75	0.51
2:R:383:ARG:NH2	2:R:434:ASP:OD1	2.44	0.51
1:F:19:ILE:O	2:R:426:VAL:HG21	2.11	0.51
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.26	0.51
2:R:356:PHE:HD2	2:R:428:ARG:HD3	1.74	0.51
2:O:478:LEU:C	2:O:478:LEU:HD23	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.10	0.51
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.92	0.50
1:A:50:LEU:O	1:A:182:ALA:HA	2.10	0.50
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.93	0.50
1:B:176:GLU:HG3	1:B:180:LYS:N	2.26	0.50
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.45	0.50
2:O:484:PRO:O	2:O:487:PRO:HD2	2.12	0.50
1:E:98:THR:OG1	1:E:101:ALA:HB3	2.11	0.50
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.46	0.50
2:N:361:HIS:H	2:N:361:HIS:CD2	2.30	0.50
2:O:376:GLU:O	2:O:442:ILE:HA	2.11	0.50
2:R:497:ASN:HD22	2:R:499:GLU:N	2.04	0.50
1:B:143:LEU:HD23	1:B:143:LEU:C	2.33	0.50
1:E:41:LYS:HD2	1:E:87:ASN:O	2.12	0.50
2:M:416:LEU:HD23	2:M:416:LEU:C	2.32	0.50
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	1.93	0.50
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.42	0.49
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.94	0.49
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.94	0.49
1:A:98:THR:O	1:A:102:GLY:HA2	2.11	0.49
1:E:176:GLU:HA	1:E:180:LYS:O	2.12	0.49
1:D:18:HIS:HD1	1:D:99:PHE:HZ	1.59	0.49
1:F:52:LEU:HD22	1:F:52:LEU:C	2.33	0.49
1:A:28:ASN:HB3	6:A:262:HOH:O	2.13	0.49
2:N:376:GLU:O	2:N:442:ILE:HA	2.12	0.49
2:M:448:PRO:HB2	2:P:516:MET:HA	1.93	0.49
1:E:31:ARG:HH11	2:Q:428:ARG:HG2	1.75	0.49
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.27	0.49
2:M:361:HIS:ND1	4:M:601:BME:H21	2.28	0.49
2:P:356:PHE:HD2	2:P:428:ARG:HD3	1.77	0.49
2:M:361:HIS:CG	4:M:601:BME:H21	2.48	0.49
2:M:491:ILE:CD1	5:M:550:4HP:H71	2.41	0.49
1:B:64:ARG:HD3	1:B:99:PHE:O	2.12	0.49
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.94	0.49
2:R:385:VAL:O	2:R:526:VAL:HA	2.12	0.49
1:B:69:GLU:HG2	1:B:94:ARG:HG2	1.95	0.48
1:C:165:GLN:H	1:C:165:GLN:CD	2.17	0.48
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.11	0.48
1:C:50:LEU:O	1:C:182:ALA:HA	2.13	0.48
1:C:98:THR:O	1:C:102:GLY:HA2	2.12	0.48
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:497:ASN:HD22	2:P:499:GLU:H	1.60	0.48
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.94	0.48
2:P:497:ASN:HD22	2:P:497:ASN:C	2.17	0.48
1:E:143:LEU:HD23	1:E:143:LEU:C	2.34	0.48
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.44	0.48
2:O:497:ASN:HD22	2:O:498:PRO:N	2.12	0.48
2:P:307:ARG:CG	2:P:533:THR:HG22	2.42	0.48
1:A:114:VAL:HG23	1:A:122:MET:HE2	1.96	0.48
1:D:18:HIS:CG	6:D:951:HOH:O	2.64	0.48
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.49	0.48
1:A:100:ASP:N	1:A:100:ASP:OD1	2.41	0.48
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.28	0.48
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.14	0.48
2:P:497:ASN:HD22	2:P:498:PRO:N	2.12	0.48
1:B:176:GLU:CG	1:B:180:LYS:N	2.77	0.47
2:O:497:ASN:HD22	2:O:499:GLU:N	2.02	0.47
2:O:491:ILE:CD1	5:O:550:4HP:H71	2.43	0.47
2:Q:473:LYS:NZ	6:Q:1135:HOH:O	2.43	0.47
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	1.96	0.47
2:Q:491:ILE:HD11	5:Q:550:4HP:H71	1.95	0.47
1:F:54:GLN:HG3	1:F:184:ARG:HH21	1.79	0.47
1:F:80:GLN:O	1:F:91:SER:HB2	2.14	0.47
2:R:449:TRP:CE3	5:R:550:4HP:H72	2.49	0.47
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.97	0.47
2:R:497:ASN:HA	2:R:498:PRO:HD2	1.77	0.47
1:D:163:GLN:HB3	1:D:165:GLN:HE22	1.79	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.75	0.47
1:A:143:LEU:HD23	1:A:143:LEU:C	2.35	0.47
1:C:99:PHE:CE2	2:O:411:LYS:HD2	2.49	0.47
2:R:416:LEU:HD23	2:R:416:LEU:C	2.34	0.47
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.49	0.47
2:M:361:HIS:N	2:M:361:HIS:CD2	2.71	0.47
2:O:473:LYS:HD2	2:O:474:LEU:N	2.28	0.47
2:P:359:HIS:O	2:P:366:ASN:HB3	2.15	0.47
1:D:5:LEU:O	2:P:387:GLN:HG2	2.14	0.47
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.77	0.47
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.50	0.47
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.33	0.47
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.97	0.47
1:F:64:ARG:O	1:F:99:PHE:HD1	1.98	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.50	0.47
2:M:362:ASP:CG	2:M:440:ARG:HD2	2.35	0.47
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.48	0.47
2:P:449:TRP:CE3	5:P:550:4HP:H72	2.50	0.47
1:B:176:GLU:OE2	1:B:179:GLY:C	2.54	0.46
1:D:143:LEU:HD23	1:D:143:LEU:C	2.36	0.46
1:E:51:LEU:HD11	1:E:126:ILE:CD1	2.45	0.46
1:E:147:ASP:OD2	1:E:174:ARG:NH1	2.49	0.46
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.50	0.46
2:R:399:MET:HA	2:R:462:HIS:O	2.16	0.46
1:B:50:LEU:O	1:B:182:ALA:HA	2.16	0.46
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.87	0.46
2:P:364:LEU:CD1	2:P:442:ILE:HG23	2.43	0.46
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.13	0.46
1:F:165:GLN:CD	1:F:165:GLN:N	2.60	0.46
2:R:306:SER:CB	2:R:530:GLN:HE21	2.27	0.46
1:C:51:LEU:HD11	1:C:126:ILE:CD1	2.45	0.46
1:E:50:LEU:O	1:E:182:ALA:HA	2.16	0.46
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.31	0.46
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.98	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.46
1:D:51:LEU:O	1:D:105:THR:HA	2.15	0.46
2:N:400:TRP:HA	2:N:425:GLY:O	2.16	0.46
1:F:40:ALA:HB2	1:F:89:PHE:HD1	1.81	0.46
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.80	0.45
1:C:63:VAL:HG12	1:C:66:SER:HB3	1.98	0.45
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.80	0.45
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.77	0.45
2:M:438:SER:O	4:M:601:BME:H22	2.16	0.45
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.71	0.45
2:R:356:PHE:CD2	2:R:428:ARG:HD3	2.51	0.45
1:B:4:LEU:HB3	2:N:387:GLN:HB3	1.97	0.45
2:O:416:LEU:C	2:O:416:LEU:HD23	2.36	0.45
1:F:133:ARG:HG3	2:R:326:THR:HG21	1.99	0.45
1:D:51:LEU:HD11	1:D:126:ILE:CD1	2.46	0.45
1:E:38:ARG:HG3	1:E:107:HIS:HB2	1.97	0.45
1:E:168:GLU:HA	1:E:171:ILE:CD1	2.36	0.45
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.98	0.45
2:R:413:ASP:C	2:R:414:ARG:HD2	2.37	0.45
1:C:114:VAL:HG23	1:C:122:MET:HE2	1.98	0.45
1:F:39:LEU:HD11	1:F:93:GLY:HA3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.52	0.45
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.98	0.45
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.99	0.45
2:O:363:LEU:HD11	2:O:427:GLY:HA3	1.99	0.45
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.83	0.45
1:C:191:GLY:O	1:C:194:GLU:HB2	2.17	0.45
1:F:174:ARG:HE	1:F:181:THR:HG23	1.81	0.45
2:P:503:GLN:HG2	6:P:648:HOH:O	2.17	0.45
1:A:165:GLN:NE2	1:C:61:HIS:NE2	2.65	0.45
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.17	0.45
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.66	0.45
2:Q:399:MET:HA	2:Q:462:HIS:O	2.17	0.45
2:R:386:ASP:HA	2:R:527:LEU:O	2.17	0.45
2:R:484:PRO:O	2:R:488:MET:CE	2.65	0.45
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.47	0.45
1:E:52:LEU:CD2	1:E:184:ARG:NH1	2.80	0.45
2:O:400:TRP:HA	2:O:425:GLY:O	2.17	0.45
1:B:39:LEU:HD11	1:B:93:GLY:HA3	2.00	0.44
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.99	0.44
2:Q:364:LEU:HD22	2:Q:440:ARG:HG2	1.99	0.44
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	3.05	0.44
1:A:114:VAL:HG23	1:A:122:MET:CE	2.48	0.44
1:A:163:GLN:HB2	6:A:269:HOH:O	2.16	0.44
1:D:50:LEU:O	1:D:182:ALA:HA	2.17	0.44
1:E:64:ARG:O	1:E:99:PHE:HD1	2.01	0.44
1:F:163:GLN:CA	1:F:165:GLN:HE22	2.30	0.44
1:E:44:ALA:O	1:E:48:HIS:NE2	2.29	0.44
1:F:177:VAL:O	1:F:180:LYS:HB3	2.17	0.44
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.52	0.44
2:O:505:ILE:HG22	2:O:507:LYS:HE2	1.98	0.44
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.76	0.44
2:Q:478:LEU:HD12	2:Q:523:PHE:CD2	2.53	0.44
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.53	0.44
1:C:114:VAL:HG23	1:C:122:MET:CE	2.48	0.44
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.81	0.44
1:F:157:VAL:O	1:F:160:LEU:HB2	2.18	0.44
2:N:478:LEU:HD12	2:N:523:PHE:CG	2.52	0.44
2:O:364:LEU:HB2	2:O:440:ARG:HD3	1.99	0.44
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.99	0.44
1:E:100:ASP:OD1	1:E:100:ASP:N	2.34	0.44
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.89	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.72	0.44
2:P:416:LEU:HD23	2:P:416:LEU:C	2.39	0.44
1:C:52:LEU:HD22	1:C:52:LEU:C	2.38	0.44
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.98	0.44
2:M:399:MET:HA	2:M:462:HIS:O	2.18	0.43
1:E:52:LEU:HA	1:E:104:TRP:O	2.18	0.43
2:M:400:TRP:HA	2:M:425:GLY:O	2.18	0.43
1:B:163:GLN:HA	1:B:164:PRO:HD2	1.65	0.43
1:D:58:GLY:HA2	1:D:190:GLN:HB3	2.00	0.43
1:E:19:ILE:HD11	2:Q:408:TYR:HD2	1.82	0.43
2:M:359:HIS:O	2:M:366:ASN:HB3	2.19	0.43
1:A:131:PHE:CE2	2:M:475:ILE:HD12	2.53	0.43
2:O:392:VAL:HG12	2:O:395:THR:HB	2.01	0.43
1:F:143:LEU:HD23	1:F:143:LEU:C	2.38	0.43
2:M:335:ALA:HB1	2:O:325:LYS:HD3	2.00	0.43
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.82	0.43
1:A:199:ASP:O	2:M:338:SER:HA	2.19	0.43
2:P:484:PRO:O	2:P:488:MET:CE	2.67	0.43
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.43
2:R:484:PRO:O	2:R:488:MET:HE3	2.17	0.43
1:B:66:SER:HB2	1:B:130:LEU:HD11	2.01	0.43
1:D:164:PRO:N	1:D:165:GLN:NE2	2.65	0.43
1:E:115:ASN:HA	1:E:121:PRO:HA	2.01	0.43
2:N:420:ASP:HA	2:N:421:PRO:HD2	1.83	0.43
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.18	0.43
2:R:348:GLY:HA3	6:R:1270:HOH:O	2.19	0.43
2:N:307:ARG:HG2	2:N:533:THR:HG22	2.00	0.42
2:O:361:HIS:CD2	6:O:708:HOH:O	2.71	0.42
2:Q:447:TYR:HA	2:Q:448:PRO:HD3	1.92	0.42
1:C:44:ALA:HA	1:C:45:PRO:HD3	1.91	0.42
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.19	0.42
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.39	0.42
1:F:4:LEU:HB3	2:R:387:GLN:HB3	2.01	0.42
1:D:172:ALA:HB1	1:D:183:TYR:HB3	2.01	0.42
1:D:84:ASN:O	1:D:87:ASN:HB2	2.19	0.42
2:P:399:MET:HA	2:P:462:HIS:O	2.19	0.42
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.54	0.42
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.19	0.42
2:M:522:ARG:HE	2:M:524:ASP:CG	2.21	0.42
2:N:497:ASN:HD22	2:N:497:ASN:C	2.21	0.42
2:O:383:ARG:HA	2:O:435:GLY:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.55	0.42
1:C:132:ALA:HB3	1:C:135:ILE:HD12	2.00	0.42
1:C:163:GLN:HA	1:C:164:PRO:HD3	1.86	0.42
1:E:165:GLN:H	1:E:165:GLN:HE21	0.65	0.42
2:P:505:ILE:HG22	2:P:507:LYS:HE3	2.01	0.42
2:M:328:ILE:HD12	2:N:335:ALA:HB2	2.02	0.42
2:R:376:GLU:O	2:R:442:ILE:HA	2.18	0.42
1:B:100:ASP:CG	1:B:101:ALA:H	2.22	0.42
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.55	0.42
2:Q:478:LEU:HD12	2:Q:523:PHE:CG	2.54	0.42
1:B:98:THR:O	1:B:102:GLY:HA2	2.19	0.42
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.62	0.42
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.93	0.42
2:O:361:HIS:HD2	2:O:361:HIS:H	1.62	0.42
2:P:392:VAL:HG12	2:P:395:THR:HB	2.01	0.42
1:A:176:GLU:HG3	1:A:180:LYS:C	2.40	0.42
1:A:20:GLY:C	1:A:21:LEU:HD23	2.41	0.42
1:F:176:GLU:OE2	1:F:179:GLY:C	2.58	0.42
2:N:414:ARG:CA	2:N:414:ARG:NE	2.80	0.42
6:F:1371:HOH:O	2:R:301:PRO:HB2	2.19	0.42
1:C:176:GLU:HG3	1:C:180:LYS:O	2.20	0.42
1:C:85:LEU:HD23	1:C:85:LEU:HA	1.93	0.42
2:M:486:ILE:HB	2:M:487:PRO:HD3	2.02	0.42
2:P:486:ILE:HB	2:P:487:PRO:HD3	2.02	0.42
2:Q:493:LYS:HE3	2:Q:493:LYS:HB2	1.81	0.42
1:E:168:GLU:CA	1:E:171:ILE:HD12	2.39	0.41
2:O:495:ILE:CG2	2:O:500:ALA:HB3	2.50	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.85	0.41
1:F:120:VAL:HA	1:F:121:PRO:HD2	1.89	0.41
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.55	0.41
1:A:110:LYS:NZ	1:A:148:GLU:OE2	2.44	0.41
1:F:85:LEU:HA	1:F:85:LEU:HD23	1.87	0.41
1:F:146:ASP:OD1	1:F:174:ARG:HB2	2.20	0.41
1:F:200:PHE:CD1	2:R:345:GLU:HG2	2.54	0.41
2:Q:486:ILE:N	2:Q:487:PRO:CD	2.83	0.41
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.85	0.41
2:P:363:LEU:HD23	2:P:425:GLY:HA2	2.02	0.41
2:R:447:TYR:OH	5:R:550:4HP:C5	2.68	0.41
1:F:52:LEU:CD2	1:F:52:LEU:C	2.89	0.41
2:P:356:PHE:CD2	2:P:428:ARG:HD3	2.54	0.41
2:Q:392:VAL:HG12	2:Q:395:THR:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:CD1	2:M:349:PRO:HG3	2.56	0.41
2:M:488:MET:CE	2:P:508:LEU:HD23	2.50	0.41
2:N:497:ASN:HD22	2:N:498:PRO:N	2.19	0.41
1:B:163:GLN:C	1:B:165:GLN:HE22	2.24	0.41
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.62	0.41
2:R:437:TYR:C	2:R:437:TYR:CD1	2.94	0.41
1:C:64:ARG:HB3	1:C:99:PHE:HA	2.03	0.41
2:M:360:ASP:HB3	2:M:428:ARG:HG3	2.03	0.41
2:N:536:GLU:HB2	6:N:703:HOH:O	2.20	0.41
2:O:362:ASP:OD1	2:O:364:LEU:HB2	2.20	0.41
2:O:495:ILE:HG21	2:O:500:ALA:HB3	2.02	0.41
2:P:430:LEU:HA	2:P:430:LEU:HD12	1.97	0.41
2:R:392:VAL:HG12	2:R:395:THR:HB	2.03	0.41
1:B:23:LEU:N	1:B:23:LEU:HD12	2.36	0.41
1:C:143:LEU:HD23	1:C:143:LEU:C	2.41	0.41
1:D:70:VAL:HG11	1:D:106:LEU:CD2	2.49	0.41
2:R:483:ASP:HA	2:R:484:PRO:HD2	1.97	0.41
2:M:447:TYR:OH	5:M:550:4HP:C5	2.70	0.40
2:N:416:LEU:C	2:N:416:LEU:CD2	2.90	0.40
2:N:356:PHE:HD1	2:N:428:ARG:HD3	1.86	0.40
2:M:522:ARG:NE	2:M:524:ASP:OD1	2.47	0.40
2:O:359:HIS:O	2:O:366:ASN:HB3	2.22	0.40
2:R:326:THR:HG22	2:R:330:ARG:HD2	2.04	0.40
1:A:191:GLY:O	1:A:194:GLU:HB2	2.21	0.40
1:A:165:GLN:NE2	1:C:61:HIS:CE1	2.90	0.40
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.21	0.40
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.57	0.40
2:P:473:LYS:HE3	2:P:475:ILE:HG13	2.02	0.40
1:F:31:ARG:HH12	2:R:428:ARG:HG2	1.84	0.40
1:E:78:GLU:OE1	6:E:239:HOH:O	2.22	0.40
1:F:177:VAL:N	1:F:180:LYS:O	2.40	0.40
2:O:363:LEU:HD23	2:O:425:GLY:CA	2.51	0.40
1:D:176:GLU:CG	1:D:179:GLY:HA2	2.51	0.40
2:O:486:ILE:N	2:O:487:PRO:CD	2.84	0.40
2:P:522:ARG:NE	2:P:524:ASP:OD1	2.49	0.40
2:R:372:LEU:HA	2:R:372:LEU:HD12	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	194 (98%)	4 (2%)	0	100	100
1	B	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	193 (98%)	4 (2%)	1 (0%)	29	17
1	E	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
1	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	R	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
All	All	2562/2628 (98%)	2484 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	100	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	154 (95%)	8 (5%)	25	12
1	B	162/163 (99%)	156 (96%)	6 (4%)	34	22
1	C	162/163 (99%)	154 (95%)	8 (5%)	25	12
1	D	162/163 (99%)	156 (96%)	6 (4%)	34	22
1	E	162/163 (99%)	156 (96%)	6 (4%)	34	22
1	F	162/163 (99%)	157 (97%)	5 (3%)	40	28
2	M	196/202 (97%)	184 (94%)	12 (6%)	18	7
2	N	196/202 (97%)	183 (93%)	13 (7%)	16	6
2	O	196/202 (97%)	184 (94%)	12 (6%)	18	7
2	P	196/202 (97%)	187 (95%)	9 (5%)	27	14
2	Q	196/202 (97%)	188 (96%)	8 (4%)	30	18
2	R	196/202 (97%)	188 (96%)	8 (4%)	30	18
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	26	13

All (101) 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	43	ASP
1	A	52	LEU
1	A	133	ARG
1	A	165	GLN
1	A	184	ARG
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	411	LYS
2	M	416	LEU
2	M	433	SER
2	M	434	ASP
2	M	440	ARG
2	M	497	ASN
2	M	503	GLN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	38	ARG
1	B	52	LEU
1	B	133	ARG
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	428	ARG
2	N	433	SER
2	N	440	ARG
2	N	478	LEU
2	N	497	ASN
2	N	507	LYS
2	N	512	ASN
2	N	534	HIS
1	C	4	LEU
1	C	9	PRO
1	C	19	ILE
1	C	38	ARG
1	C	47	GLU
1	C	52	LEU
1	C	94	ARG
1	C	165	GLN
2	O	306	SER
2	O	324	TYR
2	O	372	LEU
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	434	ASP
2	O	473	LYS
2	O	478	LEU
2	O	497	ASN
2	O	503	GLN
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	180	LYS
2	P	364	LEU
2	P	395	THR
2	P	411	LYS
2	P	416	LEU
2	P	434	ASP
2	P	440	ARG
2	P	478	LEU
2	P	497	ASN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU
1	E	165	GLN
1	E	180	LYS
2	Q	372	LEU
2	Q	395	THR
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	497	ASN
2	Q	507	LYS
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	38	ARG
1	F	52	LEU
1	F	165	GLN
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP
2	R	497	ASN
2	R	507	LYS
2	R	512	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	361	HIS
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	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	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	497	ASN
2	Q	503	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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	4HP	P	550	3	8,11,11	0.97	0	10,14,14	0.79	0
5	4HP	R	550	3	8,11,11	0.87	0	10,14,14	0.76	0
5	4HP	N	550	3	8,11,11	1.08	0	10,14,14	0.78	0
4	BME	P	601	2	3,3,3	0.44	0	1,2,2	0.59	0
4	BME	Q	601	2	3,3,3	0.70	0	1,2,2	0.09	0
4	BME	R	601	2	3,3,3	0.63	0	1,2,2	1.59	0
4	BME	M	601	2	3,3,3	0.99	0	1,2,2	0.83	0
4	BME	N	601	2	3,3,3	0.24	0	1,2,2	0.01	0
4	BME	O	601	2	3,3,3	0.52	0	1,2,2	0.03	0
5	4HP	Q	550	3	8,11,11	1.18	1 (12%)	10,14,14	1.26	1 (10%)
5	4HP	M	550	3	8,11,11	0.88	0	10,14,14	0.99	0
5	4HP	O	550	3	8,11,11	0.90	0	10,14,14	0.69	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	4HP	P	550	3	-	0/2/4/4	0/1/1/1
5	4HP	R	550	3	-	0/2/4/4	0/1/1/1
5	4HP	N	550	3	-	0/2/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
4	BME	Q	601	2	-	0/1/1/1	-
4	BME	R	601	2	-	0/1/1/1	-
4	BME	M	601	2	-	0/1/1/1	-
4	BME	N	601	2	-	1/1/1/1	-
4	BME	O	601	2	-	1/1/1/1	-
5	4HP	Q	550	3	-	0/2/4/4	0/1/1/1
5	4HP	M	550	3	-	0/2/4/4	0/1/1/1
5	4HP	O	550	3	-	0/2/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	550	4HP	C2-C1	2.56	1.44	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	550	4HP	C5-C6-C1	-2.13	118.10	121.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	601	BME	O1-C1-C2-S2
4	O	601	BME	O1-C1-C2-S2

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	550	4HP	5	0
5	R	550	4HP	3	0
5	N	550	4HP	2	0
4	Q	601	BME	1	0
4	M	601	BME	3	0
4	O	601	BME	1	0
5	Q	550	4HP	2	0
5	M	550	4HP	4	0
5	O	550	4HP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.