Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 02:08 PM EDT

PDB ID	:	3PCA
Title	:	STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COMPLEXED WITH 3,4-DIHYDROXYBENZOATE
Authors	:	Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on	:	1997-07-18
Resolution	:	2.20 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

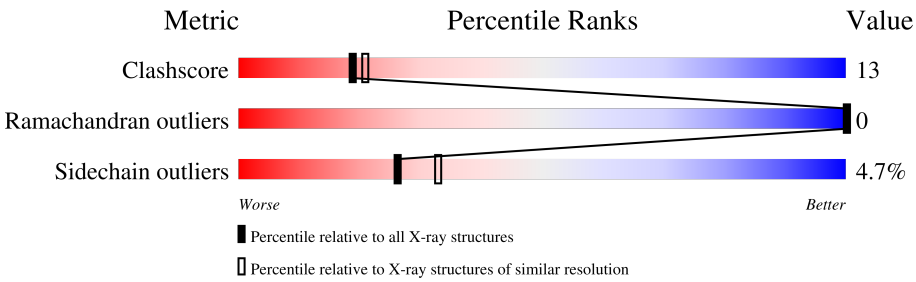
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	72% 24% •
1	B	200	73% 21% 5% •
1	C	200	70% 24% • •
1	D	200	70% 25% • •
1	E	200	65% 30% •
1	F	200	68% 26% 6%
2	M	238	69% 25% • •
2	N	238	73% 21% • •

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Mol	Chain	Length	Quality of chain
2	O	238	70% 24%
2	P	238	71% 22%
2	Q	238	71% 23%
2	R	238	70% 21% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22020 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
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

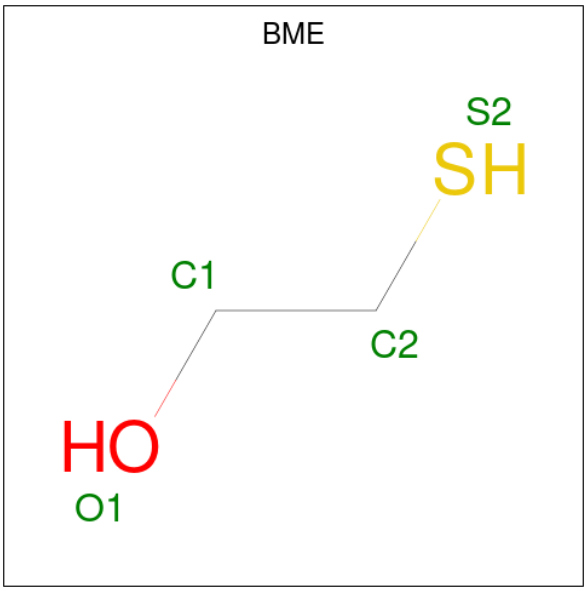
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

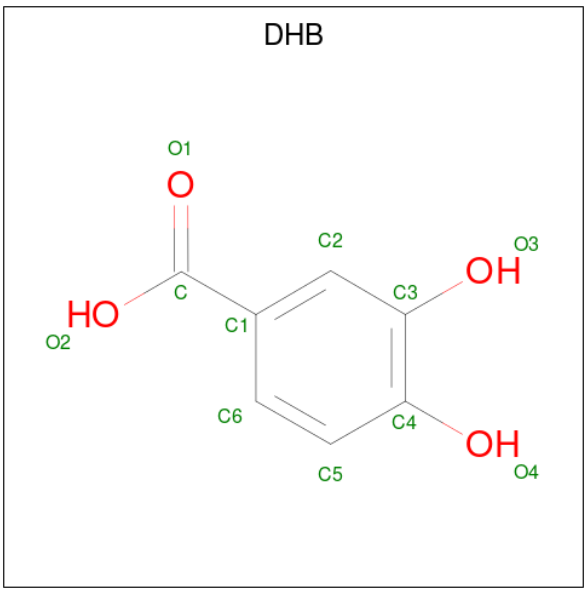
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
3	M	1	1	1	0	0
3	N	1	1	1	0	0
3	O	1	1	1	0	0
3	P	1	1	1	0	0
3	Q	1	1	1	0	0
3	R	1	1	1	0	0

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



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

- Molecule 5 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	O		0	0
			11	7	4			
5	M	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	N	1	Total	C	O		0	0
			11	7	4			
5	O	1	Total	C	O		0	0
			11	7	4			
5	P	1	Total	C	O		0	0
			11	7	4			
5	P	1	Total	C	O		0	0
			11	7	4			
5	Q	1	Total	C	O		0	0
			11	7	4			
5	Q	1	Total	C	O		0	0
			11	7	4			
5	R	1	Total	C	O		0	0
			11	7	4			
5	R	1	Total	C	O		0	0
			11	7	4			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	84	84	84	0	0
			Total	O		
6	M	148	148	148	0	0
			Total	O		
6	B	78	78	78	0	0
			Total	O		
6	N	160	160	160	0	0
			Total	O		
6	C	83	83	83	0	0
			Total	O		
6	O	146	146	146	0	0
			Total	O		
6	D	76	76	76	0	0
			Total	O		
6	P	149	149	149	0	0
			Total	O		
6	E	79	79	79	0	0
			Total	O		
6	Q	156	156	156	0	0
			Total	O		
6	F	81	81	81	0	0
			Total	O		
6	R	152	152	152	0	0

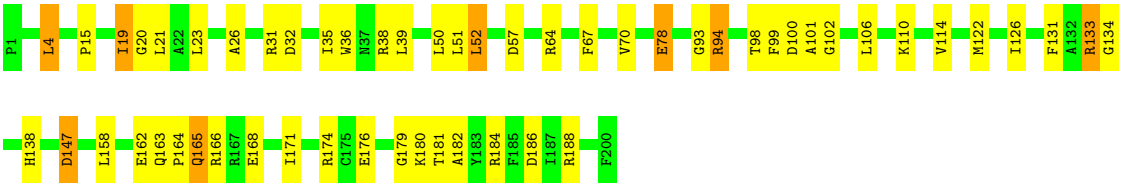
3 Residue-property plots (i)

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

Note EDS was not executed.

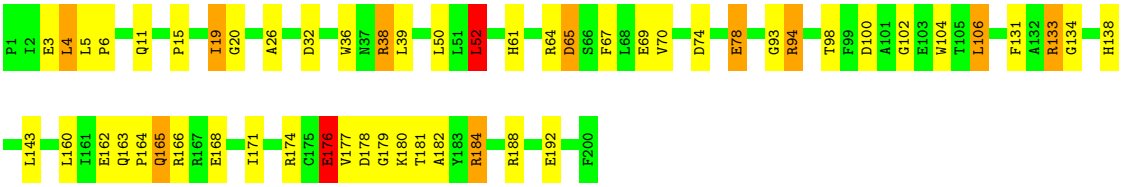
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A:



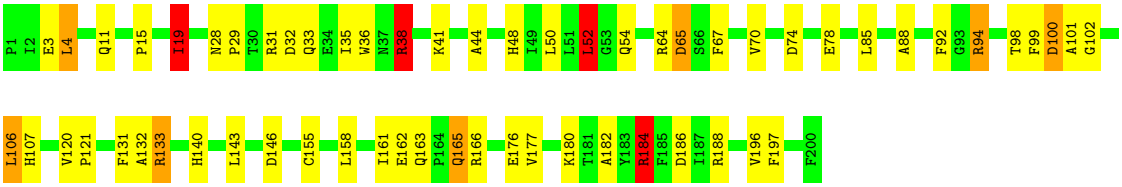
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B:



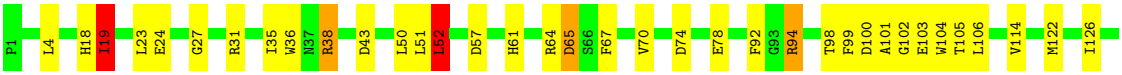
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

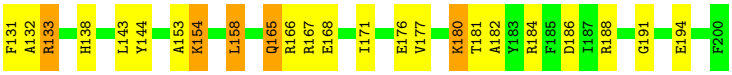
Chain C:



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

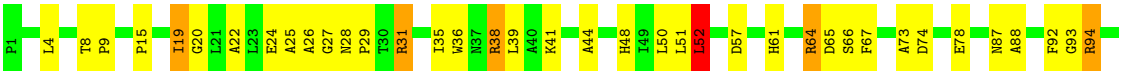
Chain D:





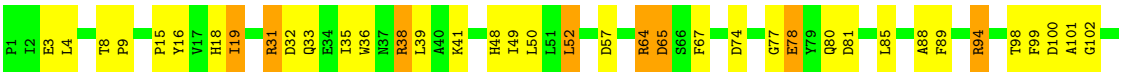
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:

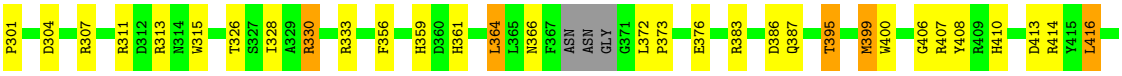


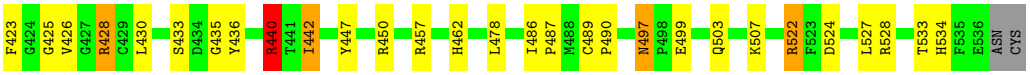
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

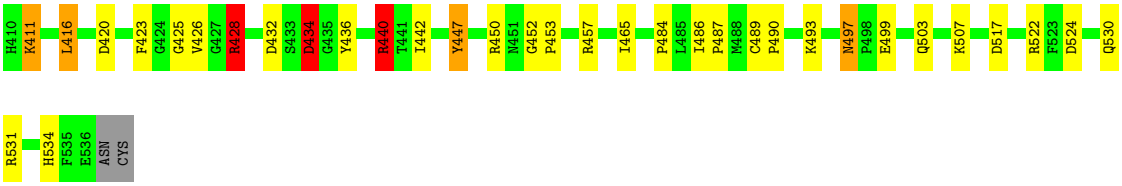
Chain N:





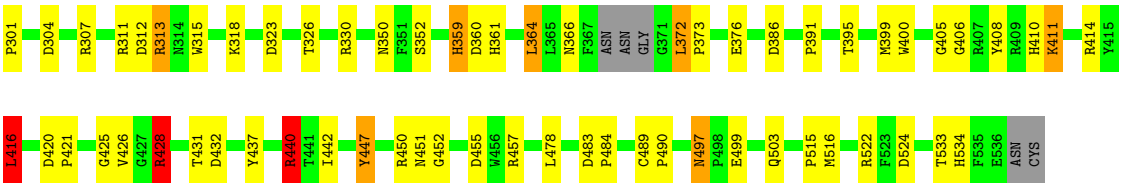
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:



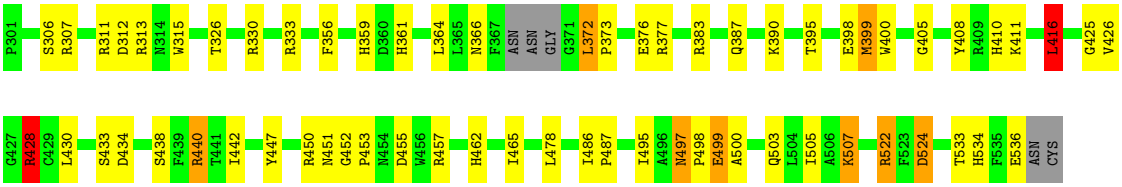
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:



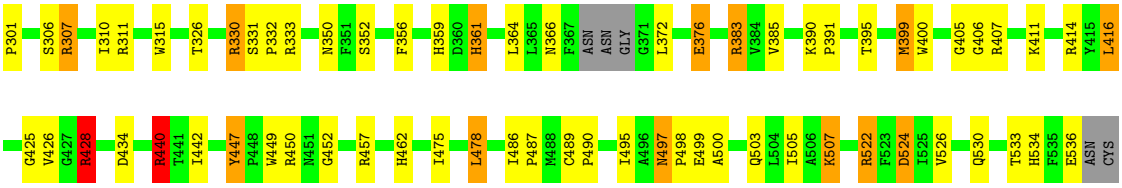
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

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 is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.30Å 127.20Å 133.80Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	96.0 (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22020	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, DHB, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	0/1611	1.56	26/2195 (1.2%)
1	B	0.92	0/1611	1.56	24/2195 (1.1%)
1	C	0.94	0/1611	1.58	22/2195 (1.0%)
1	D	0.93	1/1611 (0.1%)	1.59	25/2195 (1.1%)
1	E	0.94	0/1611	1.48	17/2195 (0.8%)
1	F	0.94	0/1611	1.57	23/2195 (1.0%)
2	M	0.97	0/1895	1.51	28/2580 (1.1%)
2	N	0.94	0/1895	1.55	19/2580 (0.7%)
2	O	0.94	0/1895	1.50	27/2580 (1.0%)
2	P	0.95	0/1895	1.54	24/2580 (0.9%)
2	Q	0.97	1/1895 (0.1%)	1.53	27/2580 (1.0%)
2	R	0.96	0/1895	1.49	24/2580 (0.9%)
All	All	0.94	2/21036 (0.0%)	1.54	286/28650 (1.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	ARG	CD-NE	-6.46	1.35	1.46
2	Q	433	SER	CB-OG	5.26	1.49	1.42

All (286) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ARG	NE-CZ-NH2	-18.94	110.83	120.30
2	R	440	ARG	NE-CZ-NH2	-18.52	111.04	120.30
2	P	440	ARG	NE-CZ-NH2	-17.63	111.49	120.30
2	N	440	ARG	NE-CZ-NH2	-17.33	111.63	120.30
2	Q	440	ARG	NE-CZ-NH2	-16.98	111.81	120.30
2	M	440	ARG	NE-CZ-NH2	-16.88	111.86	120.30
1	C	94	ARG	NE-CZ-NH1	16.86	128.73	120.30
1	D	94	ARG	NE-CZ-NH1	16.79	128.69	120.30
1	D	94	ARG	NE-CZ-NH2	-15.84	112.38	120.30
1	B	94	ARG	NE-CZ-NH1	14.60	127.60	120.30
2	O	440	ARG	NE-CZ-NH2	-13.84	113.38	120.30
1	F	142	ARG	NE-CZ-NH1	13.55	127.07	120.30
1	B	184	ARG	NE-CZ-NH2	-12.77	113.91	120.30
2	Q	457	ARG	NE-CZ-NH1	12.25	126.43	120.30
1	D	133	ARG	NE-CZ-NH2	-12.01	114.30	120.30
2	Q	428	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	B	94	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	94	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	E	133	ARG	NE-CZ-NH2	-11.39	114.61	120.30
2	N	522	ARG	CD-NE-CZ	11.36	139.51	123.60
2	N	428	ARG	NE-CZ-NH1	11.34	125.97	120.30
2	O	428	ARG	NE-CZ-NH1	10.98	125.79	120.30
2	N	313	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	O	383	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	F	94	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	C	133	ARG	NE-CZ-NH2	-10.88	114.86	120.30
2	P	440	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	94	ARG	CD-NE-CZ	10.81	138.73	123.60
1	D	94	ARG	CD-NE-CZ	10.81	138.73	123.60
2	N	457	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	94	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	C	94	ARG	CD-NE-CZ	10.38	138.13	123.60
1	D	94	ARG	CG-CD-NE	10.17	133.15	111.80
2	P	457	ARG	CD-NE-CZ	10.17	137.84	123.60
1	D	166	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	F	166	ARG	NE-CZ-NH1	9.95	125.28	120.30
2	N	450	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	A	166	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	F	94	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	B	133	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	F	133	ARG	NE-CZ-NH2	-9.61	115.50	120.30
2	Q	524	ASP	CB-CG-OD1	9.57	126.91	118.30
1	D	188	ARG	NE-CZ-NH1	9.46	125.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	ARG	NE-CZ-NH2	-9.44	115.58	120.30
2	M	313	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	P	447	TYR	CB-CG-CD2	9.23	126.54	121.00
1	C	188	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	166	ARG	NE-CZ-NH2	-9.07	115.77	120.30
2	R	428	ARG	NE-CZ-NH2	-8.99	115.80	120.30
2	O	313	ARG	NE-CZ-NH1	8.97	124.78	120.30
2	N	428	ARG	NE-CZ-NH2	-8.87	115.86	120.30
2	P	450	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	O	428	ARG	NE-CZ-NH2	-8.69	115.96	120.30
2	O	450	ARG	NE-CZ-NH1	8.66	124.63	120.30
2	Q	333	ARG	NE-CZ-NH1	8.61	124.61	120.30
2	P	428	ARG	NE-CZ-NH2	-8.58	116.01	120.30
2	P	457	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	188	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	R	524	ASP	CB-CG-OD1	8.44	125.89	118.30
2	O	517	ASP	CB-CG-OD1	8.44	125.89	118.30
1	F	142	ARG	NE-CZ-NH2	-8.43	116.09	120.30
2	R	428	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	D	184	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	P	414	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	E	52	LEU	CB-CA-C	8.29	125.95	110.20
2	P	447	TYR	CB-CG-CD1	-8.28	116.03	121.00
2	Q	330	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	D	133	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	C	166	ARG	NE-CZ-NH1	8.21	124.40	120.30
2	O	457	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	F	31	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	N	522	ARG	NE-CZ-NH1	8.08	124.34	120.30
2	N	440	ARG	NE-CZ-NH1	8.05	124.33	120.30
2	P	524	ASP	CB-CG-OD1	8.03	125.53	118.30
1	F	188	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	F	188	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	E	166	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	188	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	A	31	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	M	457	ARG	CD-NE-CZ	7.83	134.57	123.60
2	Q	457	ARG	NE-CZ-NH2	-7.82	116.39	120.30
2	N	330	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	C	186	ASP	CB-CG-OD1	7.67	125.21	118.30
1	E	31	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	D	186	ASP	CB-CG-OD1	7.53	125.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	313	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	166	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	R	450	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	R	311	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	M	428	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	M	528	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	E	38	ARG	NE-CZ-NH2	-7.37	116.61	120.30
2	N	333	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	133	ARG	NE-CZ-NH2	-7.33	116.64	120.30
2	R	311	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	31	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	F	74	ASP	CB-CG-OD1	7.23	124.80	118.30
2	P	428	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	E	94	ARG	NE-CZ-NH1	7.17	123.88	120.30
2	R	307	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	94	ARG	CB-CG-CD	7.15	130.19	111.60
2	N	311	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	B	36	TRP	CB-CA-C	7.12	124.63	110.40
2	M	383	ARG	NE-CZ-NH2	-7.11	116.74	120.30
2	O	531	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	Q	457	ARG	CD-NE-CZ	7.07	133.49	123.60
2	O	432	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	94	ARG	CB-CG-CD	7.02	129.85	111.60
2	P	304	ASP	CB-CG-OD1	6.99	124.59	118.30
2	O	517	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	D	65	ASP	CB-CG-OD1	6.93	124.54	118.30
2	Q	440	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	174	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	184	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	184	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	184	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	C	106	LEU	CA-CB-CG	6.79	130.91	115.30
2	M	521	TYR	CB-CG-CD1	-6.77	116.94	121.00
2	O	450	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	F	36	TRP	CB-CA-C	6.76	123.91	110.40
2	P	311	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	F	31	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	52	LEU	CB-CA-C	6.72	122.97	110.20
1	B	166	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	166	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	167	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	D	36	TRP	CB-CA-C	6.67	123.73	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	CG-CD-NE	6.66	125.79	111.80
2	O	353	HIS	CA-CB-CG	-6.66	102.28	113.60
2	P	312	ASP	CB-CG-OD1	6.65	124.29	118.30
1	E	186	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	52	LEU	CB-CA-C	6.63	122.80	110.20
1	C	133	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	R	414	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	R	376	GLU	OE1-CD-OE2	6.60	131.22	123.30
2	N	428	ARG	CG-CD-NE	6.58	125.61	111.80
2	Q	522	ARG	NE-CZ-NH1	-6.53	117.04	120.30
2	O	432	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	F	65	ASP	CB-CG-OD1	6.50	124.15	118.30
2	Q	434	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	N	528	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	78	GLU	OE1-CD-OE2	6.49	131.09	123.30
2	M	312	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	52	LEU	CB-CA-C	6.46	122.47	110.20
2	M	307	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	Q	333	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	C	36	TRP	CB-CA-C	6.35	123.11	110.40
2	O	323	ASP	CB-CG-OD1	6.35	124.01	118.30
2	O	409	ARG	NE-CZ-NH1	-6.32	117.14	120.30
2	O	531	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	23	LEU	CB-CA-C	6.30	122.18	110.20
2	Q	383	ARG	NE-CZ-NH2	-6.29	117.16	120.30
2	Q	311	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	36	TRP	CB-CA-C	6.28	122.95	110.40
1	B	188	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	E	57	ASP	CB-CG-OD1	6.27	123.94	118.30
2	P	414	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	31	ARG	CD-NE-CZ	6.26	132.37	123.60
2	R	383	ARG	NE-CZ-NH2	-6.25	117.17	120.30
2	M	524	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	188	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	Q	524	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	O	428	ARG	CD-NE-CZ	6.19	132.27	123.60
2	Q	313	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	F	52	LEU	CB-CA-C	6.17	121.92	110.20
1	C	19	ILE	CA-CB-CG1	6.15	122.68	111.00
2	N	524	ASP	CB-CG-OD1	6.12	123.81	118.30
2	Q	499	GLU	CA-CB-CG	6.12	126.85	113.40
2	R	333	ARG	NE-CZ-NH2	6.11	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	524	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	A	57	ASP	CB-CG-OD1	6.09	123.78	118.30
1	F	52	LEU	CA-CB-CG	6.08	129.28	115.30
2	P	386	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	11	GLN	N-CA-CB	6.05	121.50	110.60
1	C	146	ASP	CB-CG-OD1	6.05	123.74	118.30
2	R	457	ARG	CA-CB-CG	6.05	126.70	113.40
2	P	524	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	F	57	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	C	32	ASP	CB-CG-OD1	6.00	123.69	118.30
1	A	174	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	O	313	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	M	377	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	E	184	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	32	ASP	CB-CG-OD1	5.92	123.63	118.30
2	Q	330	ARG	NE-CZ-NH1	5.91	123.26	120.30
2	P	416	LEU	CA-CB-CG	5.89	128.85	115.30
2	R	440	ARG	NH1-CZ-NH2	5.87	125.85	119.40
1	D	57	ASP	CB-CG-OD1	5.86	123.58	118.30
2	M	428	ARG	CB-CG-CD	5.84	126.79	111.60
1	E	74	ASP	CB-CG-OD1	5.80	123.52	118.30
2	R	457	ARG	CD-NE-CZ	5.79	131.71	123.60
1	D	23	LEU	CB-CA-C	5.79	121.20	110.20
2	M	432	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	A	147	ASP	CB-CG-OD1	5.77	123.50	118.30
2	M	428	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	M	457	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	N	304	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	176	GLU	CB-CG-CD	5.75	129.71	114.20
2	M	440	ARG	NH1-CZ-NH2	5.74	125.72	119.40
2	O	524	ASP	CB-CG-OD1	5.73	123.46	118.30
2	Q	311	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	R	376	GLU	CG-CD-OE2	-5.71	106.89	118.30
2	R	522	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	F	38	ARG	CA-CB-CG	5.67	125.88	113.40
2	O	420	ASP	CB-CG-OD1	5.63	123.37	118.30
2	Q	450	ARG	CD-NE-CZ	-5.61	115.75	123.60
2	R	440	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	R	457	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	M	330	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	78	GLU	CA-CB-CG	5.57	125.66	113.40
2	M	509	ASP	CB-CG-OD1	5.57	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	377	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	D	43	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	M	312	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	52	LEU	CA-CB-CG	5.54	128.05	115.30
2	R	361	HIS	CA-CB-CG	-5.54	104.18	113.60
2	Q	452	GLY	N-CA-C	-5.54	99.25	113.10
1	D	133	ARG	N-CA-CB	-5.53	100.65	110.60
1	B	192	GLU	CA-CB-CG	5.52	125.54	113.40
1	E	64	ARG	CD-NE-CZ	-5.50	115.90	123.60
2	P	432	ASP	CB-CG-OD1	5.48	123.23	118.30
2	M	323	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	52	LEU	CB-CA-C	5.47	120.60	110.20
2	N	414	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	19	ILE	CB-CA-C	5.47	122.54	111.60
1	D	74	ASP	CB-CG-OD1	5.47	123.22	118.30
2	P	323	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	94	ARG	CD-NE-CZ	5.43	131.21	123.60
1	E	94	ARG	CG-CD-NE	5.42	123.18	111.80
1	E	64	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	E	38	ARG	CD-NE-CZ	-5.38	116.07	123.60
2	M	313	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	106	LEU	CA-CB-CG	5.37	127.65	115.30
2	O	330	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	11	GLN	N-CA-CB	5.32	120.18	110.60
1	C	133	ARG	CA-CB-CG	5.32	125.10	113.40
2	Q	383	ARG	N-CA-CB	-5.31	101.05	110.60
2	R	452	GLY	N-CA-C	-5.30	99.84	113.10
1	B	52	LEU	CA-CB-CG	5.29	127.48	115.30
1	D	103	GLU	CG-CD-OE1	-5.28	107.75	118.30
1	D	19	ILE	CB-CA-C	5.26	122.11	111.60
1	C	38	ARG	CD-NE-CZ	-5.24	116.26	123.60
2	O	330	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	O	314	ASN	CB-CA-C	5.24	120.87	110.40
1	F	64	ARG	CD-NE-CZ	-5.23	116.27	123.60
1	D	38	ARG	CD-NE-CZ	-5.23	116.28	123.60
2	O	447	TYR	N-CA-CB	-5.22	101.19	110.60
1	F	133	ARG	CA-CB-CG	5.22	124.88	113.40
1	B	74	ASP	CB-CG-OD1	5.21	122.99	118.30
1	F	78	GLU	OE1-CD-OE2	5.21	129.56	123.30
1	E	133	ARG	N-CA-CB	-5.21	101.22	110.60
2	M	447	TYR	N-CA-CB	-5.21	101.23	110.60
1	D	158	LEU	CB-CA-C	5.20	120.09	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	323	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	100	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	N	442	ILE	CA-CB-CG2	5.17	121.24	110.90
2	O	434	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	F	176	GLU	CG-CD-OE1	5.16	128.61	118.30
2	Q	416	LEU	CA-CB-CG	5.15	127.14	115.30
2	R	447	TYR	N-CA-CB	-5.14	101.35	110.60
1	B	176	GLU	OE1-CD-OE2	-5.13	117.14	123.30
2	M	452	GLY	N-CA-C	-5.13	100.29	113.10
2	R	407	ARG	CD-NE-CZ	-5.13	116.42	123.60
1	C	65	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	147	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	M	311	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	Q	312	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	176	GLU	CG-CD-OE1	5.08	128.47	118.30
2	Q	447	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	F	31	ARG	CD-NE-CZ	5.08	130.72	123.60
2	M	428	ARG	CD-NE-CZ	5.08	130.71	123.60
1	B	178	ASP	CB-CG-OD2	5.08	122.87	118.30
2	P	447	TYR	N-CA-CB	-5.07	101.48	110.60
1	F	183	TYR	CA-CB-CG	5.06	123.02	113.40
2	M	428	ARG	CG-CD-NE	5.05	122.41	111.80
1	B	65	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	94	ARG	CB-CG-CD	5.05	124.72	111.60
2	P	359	HIS	CA-CB-CG	-5.05	105.02	113.60
2	R	330	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	E	166	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	P	452	GLY	N-CA-C	-5.03	100.53	113.10
2	Q	499	GLU	CG-CD-OE1	5.03	128.35	118.30
2	O	452	GLY	N-CA-C	-5.02	100.55	113.10
1	E	186	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	M	407	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	186	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	43	0
1	B	1571	0	1499	44	0
1	C	1571	0	1499	51	0
1	D	1571	0	1499	48	0
1	E	1571	0	1499	52	0
1	F	1571	0	1499	64	0
2	M	1840	0	1793	49	0
2	N	1840	0	1793	42	0
2	O	1840	0	1793	48	0
2	P	1840	0	1793	49	0
2	Q	1840	0	1793	52	0
2	R	1840	0	1793	56	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	0	0
4	N	4	0	5	0	0
4	O	4	0	5	0	0
4	P	4	0	5	0	0
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	8	1	0
5	N	33	0	13	0	0
5	O	11	0	3	1	0
5	P	22	0	8	0	0
5	Q	22	0	9	0	0
5	R	22	0	9	0	0
6	A	84	0	0	0	0
6	B	78	0	0	0	0
6	C	83	0	0	0	0
6	D	76	0	0	0	0
6	E	79	0	0	1	0
6	F	81	0	0	1	0
6	M	148	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	160	0	0	1	0
6	O	146	0	0	6	0
6	P	149	0	0	3	0
6	Q	156	0	0	5	0
6	R	152	0	0	5	0
All	All	22020	0	19832	530	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 (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:HE21	1:E:165:GLN:N	1.38	1.19
1:E:165:GLN:H	1:E:165:GLN:NE2	1.37	1.19
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.43	1.00
1:B:165:GLN:H	1:B:165:GLN:NE2	1.61	0.98
1:F:64:ARG:NH1	1:F:100:ASP:O	1.96	0.98
2:R:497:ASN:HD22	2:R:499:GLU:H	1.13	0.95
1:D:165:GLN:H	1:D:165:GLN:HE21	1.10	0.94
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.49	0.94
1:F:165:GLN:H	1:F:165:GLN:NE2	1.65	0.93
2:Q:390:LYS:HD2	6:Q:1004:HOH:O	1.67	0.91
1:B:165:GLN:H	1:B:165:GLN:HE21	1.09	0.91
1:F:165:GLN:H	1:F:165:GLN:HE21	1.20	0.88
2:R:361:HIS:H	2:R:361:HIS:CD2	1.91	0.88
1:D:64:ARG:NH1	1:D:100:ASP:O	2.08	0.87
1:B:70:VAL:HG11	1:B:106:LEU:HD21	1.55	0.87
1:D:165:GLN:H	1:D:165:GLN:NE2	1.73	0.86
1:A:98:THR:HB	1:A:100:ASP:OD1	1.75	0.85
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.57	0.85
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.59	0.85
2:R:497:ASN:ND2	2:R:499:GLU:H	1.76	0.84
1:A:70:VAL:HG11	1:A:106:LEU:HD21	1.62	0.82
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.45	0.81
1:C:64:ARG:NH1	1:C:100:ASP:O	2.13	0.81
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.45	0.81
1:E:180:LYS:HG3	1:E:181:THR:N	1.96	0.80
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.01	0.78
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.63	0.78
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ILE:O	2:P:426:VAL:HG21	1.85	0.76
2:O:497:ASN:HD22	2:O:499:GLU:H	1.31	0.75
2:O:361:HIS:H	2:O:361:HIS:CD2	2.05	0.75
1:C:165:GLN:H	1:C:165:GLN:NE2	1.85	0.75
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.50	0.75
1:F:19:ILE:O	2:R:426:VAL:HG21	1.88	0.74
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.03	0.74
2:M:361:HIS:H	2:M:361:HIS:CD2	2.05	0.73
1:D:165:GLN:HE21	1:D:165:GLN:N	1.86	0.73
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.52	0.73
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.68	0.73
1:E:64:ARG:NH1	1:E:100:ASP:O	2.21	0.73
1:B:165:GLN:HE21	1:B:165:GLN:N	1.85	0.73
2:M:390:LYS:HD2	6:M:638:HOH:O	1.89	0.72
2:N:497:ASN:HD22	2:N:499:GLU:H	1.38	0.72
2:M:497:ASN:ND2	2:M:499:GLU:H	1.86	0.71
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.54	0.71
1:B:176:GLU:HG3	1:B:180:LYS:O	1.91	0.71
1:D:180:LYS:HG3	1:D:181:THR:N	2.07	0.70
2:M:522:ARG:NH1	6:M:660:HOH:O	2.24	0.70
2:M:497:ASN:HD22	2:M:499:GLU:H	1.39	0.70
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.39	0.70
2:R:497:ASN:HD22	2:R:499:GLU:N	1.88	0.69
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.26	0.69
2:P:497:ASN:HD22	2:P:499:GLU:H	1.40	0.69
1:A:64:ARG:NH1	1:A:100:ASP:O	2.27	0.68
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.24	0.67
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.94	0.67
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.23	0.67
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.30	0.67
1:C:70:VAL:HG11	1:C:106:LEU:HD21	1.77	0.67
1:A:176:GLU:HG3	1:A:180:LYS:O	1.95	0.66
2:Q:522:ARG:NH1	6:Q:1040:HOH:O	2.28	0.66
2:P:361:HIS:H	2:P:361:HIS:CD2	2.14	0.66
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.95	0.66
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.61	0.66
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.78	0.66
2:P:376:GLU:OE1	6:P:642:HOH:O	2.12	0.66
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.27	0.66
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.77	0.66
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:HG2	2:O:301:PRO:CG	2.27	0.65
1:F:48:HIS:C	1:F:180:LYS:HZ2	1.99	0.65
2:R:361:HIS:H	2:R:361:HIS:HD2	1.38	0.65
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.42	0.65
2:P:313:ARG:O	2:P:318:LYS:HE2	1.95	0.65
1:D:70:VAL:HG11	1:D:106:LEU:HD21	1.78	0.65
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.77	0.65
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.44	0.65
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.31	0.65
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.30	0.65
2:O:497:ASN:ND2	2:O:499:GLU:H	1.95	0.64
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.32	0.64
2:N:361:HIS:CD2	2:N:361:HIS:H	2.15	0.64
2:O:406:GLY:O	2:O:447:TYR:HD1	1.81	0.64
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.28	0.64
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.13	0.64
1:B:64:ARG:NH1	1:B:100:ASP:O	2.30	0.64
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.13	0.64
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.80	0.64
1:A:134:GLY:HA3	2:M:326:THR:HG22	1.80	0.64
2:P:326:THR:HG22	2:P:330:ARG:HD2	1.79	0.64
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.95	0.64
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.45	0.63
1:C:44:ALA:O	1:C:48:HIS:NE2	2.28	0.63
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.24	0.63
2:Q:359:HIS:O	2:Q:366:ASN:HB3	1.99	0.63
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.26	0.62
1:B:134:GLY:HA3	2:N:326:THR:HG22	1.82	0.62
1:E:98:THR:HB	1:E:100:ASP:OD1	2.00	0.62
2:R:536:GLU:HB2	6:R:1315:HOH:O	1.98	0.62
2:N:497:ASN:ND2	2:N:499:GLU:H	1.98	0.62
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.29	0.62
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.82	0.62
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.81	0.62
1:F:50:LEU:O	1:F:182:ALA:HA	1.99	0.62
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	1.97	0.61
1:D:78:GLU:HG2	2:P:301:PRO:CB	2.31	0.61
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.83	0.60
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	1.99	0.60
1:B:98:THR:O	1:B:102:GLY:HA2	2.01	0.60
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASP:OD1	1:C:100:ASP:N	2.34	0.60
1:D:78:GLU:HG2	2:P:301:PRO:HB3	1.83	0.60
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.02	0.60
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.15	0.60
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.66	0.60
1:C:177:VAL:O	1:C:180:LYS:HB3	2.02	0.60
1:B:176:GLU:HG3	1:B:180:LYS:C	2.22	0.60
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.31	0.60
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.83	0.60
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.36	0.59
2:Q:536:GLU:HB2	6:Q:1083:HOH:O	2.01	0.59
1:F:78:GLU:HG2	2:R:301:PRO:CB	2.31	0.59
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.84	0.59
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.82	0.59
1:C:19:ILE:HD11	2:O:408:TYR:HD2	1.68	0.59
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.67	0.58
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.20	0.58
2:P:497:ASN:ND2	2:P:499:GLU:H	2.01	0.58
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.19	0.58
2:R:405:GLY:HA3	6:R:1240:HOH:O	2.03	0.58
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.84	0.58
2:M:361:HIS:H	2:M:361:HIS:HD2	1.45	0.58
1:E:29:PRO:O	6:E:266:HOH:O	2.17	0.58
1:F:176:GLU:OE2	1:F:179:GLY:HA2	2.03	0.58
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.39	0.57
1:D:143:LEU:C	1:D:143:LEU:HD23	2.24	0.57
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.86	0.57
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.86	0.57
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.52	0.57
1:D:19:ILE:HG21	2:P:410:HIS:HB2	1.86	0.57
1:C:78:GLU:HG2	2:O:301:PRO:HG2	1.86	0.57
2:O:522:ARG:NH1	6:O:670:HOH:O	2.26	0.57
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.04	0.57
1:A:176:GLU:HA	1:A:180:LYS:O	2.04	0.57
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.20	0.57
1:F:77:GLY:O	1:F:114:VAL:HG12	2.05	0.57
2:R:522:ARG:NE	2:R:524:ASP:OD1	2.36	0.57
2:M:310:ILE:HD12	2:O:453:PRO:HB2	1.87	0.56
2:P:361:HIS:H	2:P:361:HIS:HD2	1.52	0.56
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.86	0.56
1:F:165:GLN:HE21	1:F:165:GLN:N	1.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:390:LYS:HD3	6:R:1236:HOH:O	2.05	0.56
2:N:364:LEU:CD2	2:N:440:ARG:HD3	2.32	0.56
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.06	0.56
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.68	0.56
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.86	0.56
2:M:497:ASN:HD22	2:M:497:ASN:C	2.09	0.56
2:M:497:ASN:HD22	2:M:498:PRO:N	2.04	0.56
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.87	0.56
2:O:390:LYS:HD2	6:O:649:HOH:O	2.06	0.55
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.88	0.55
1:B:133:ARG:NH2	1:C:162:GLU:OE2	2.39	0.55
1:C:165:GLN:H	1:C:165:GLN:HE21	1.52	0.55
1:E:114:VAL:HG23	1:E:122:MET:CE	2.37	0.55
1:D:99:PHE:HE2	2:P:411:LYS:HD2	1.71	0.55
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.55
1:F:177:VAL:O	1:F:180:LYS:HB3	2.07	0.55
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.88	0.55
1:F:98:THR:HB	1:F:100:ASP:OD1	2.06	0.55
1:D:100:ASP:OD1	1:D:100:ASP:N	2.38	0.55
1:D:191:GLY:O	1:D:194:GLU:HB2	2.06	0.55
1:D:51:LEU:O	1:D:105:THR:HA	2.06	0.55
1:F:64:ARG:HD3	1:F:99:PHE:O	2.07	0.55
1:A:165:GLN:CD	1:A:165:GLN:H	2.10	0.55
1:C:50:LEU:O	1:C:182:ALA:HA	2.06	0.54
1:F:48:HIS:C	1:F:180:LYS:NZ	2.60	0.54
2:R:361:HIS:CD2	2:R:361:HIS:N	2.65	0.54
2:R:390:LYS:HE2	6:R:1352:HOH:O	2.07	0.54
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.89	0.54
2:M:399:MET:HA	2:M:462:HIS:O	2.08	0.54
2:N:400:TRP:HA	2:N:425:GLY:O	2.08	0.54
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.07	0.54
1:B:98:THR:HB	1:B:100:ASP:OD1	2.08	0.54
2:N:361:HIS:H	2:N:361:HIS:HD2	1.54	0.54
1:F:180:LYS:HD2	1:F:181:THR:N	2.22	0.54
1:E:98:THR:O	1:E:102:GLY:HA2	2.07	0.54
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.89	0.53
1:A:70:VAL:HG11	1:A:106:LEU:CD2	2.37	0.53
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.24	0.53
2:O:361:HIS:H	2:O:361:HIS:HD2	1.52	0.53
1:E:31:ARG:NH1	2:Q:428:ARG:HG2	2.23	0.53
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:406:GLY:O	2:O:447:TYR:CD1	2.61	0.53
2:P:405:GLY:HA3	6:P:651:HOH:O	2.08	0.53
2:R:400:TRP:HA	2:R:425:GLY:O	2.09	0.53
1:C:163:GLN:HB3	1:C:165:GLN:NE2	2.23	0.53
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.44	0.53
2:R:399:MET:HA	2:R:462:HIS:O	2.08	0.53
1:C:15:PRO:HB3	1:C:133:ARG:HD2	1.91	0.53
2:Q:453:PRO:CB	2:R:310:ILE:HD12	2.34	0.53
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.43	0.52
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.13	0.52
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.97	0.52
1:C:176:GLU:HG3	1:C:180:LYS:O	2.09	0.52
1:C:38:ARG:HG3	1:C:107:HIS:HB2	1.91	0.52
1:B:78:GLU:HG2	2:N:301:PRO:HB3	1.92	0.52
2:O:390:LYS:HE2	6:O:722:HOH:O	2.10	0.52
1:F:98:THR:OG1	1:F:102:GLY:N	2.43	0.52
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.45	0.52
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.45	0.52
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.45	0.51
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.07	0.51
2:N:376:GLU:O	2:N:442:ILE:HA	2.09	0.51
1:E:133:ARG:HG2	2:Q:326:THR:HG21	1.91	0.51
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.46	0.51
1:F:99:PHE:HE2	2:R:411:LYS:HD3	1.76	0.51
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.36	0.51
2:Q:399:MET:HA	2:Q:462:HIS:O	2.10	0.51
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.93	0.51
1:D:19:ILE:CG2	2:P:410:HIS:HB2	2.40	0.51
1:B:50:LEU:O	1:B:182:ALA:HA	2.11	0.51
1:D:98:THR:O	1:D:102:GLY:HA2	2.10	0.51
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.92	0.51
1:F:143:LEU:C	1:F:143:LEU:HD23	2.31	0.51
2:R:406:GLY:O	2:R:447:TYR:HD1	1.94	0.51
2:N:359:HIS:O	2:N:366:ASN:HB3	2.11	0.51
1:F:99:PHE:CE2	2:R:411:LYS:HD3	2.46	0.51
1:F:176:GLU:OE2	1:F:179:GLY:C	2.49	0.51
2:P:400:TRP:HA	2:P:425:GLY:O	2.11	0.51
1:E:176:GLU:HA	1:E:180:LYS:O	2.10	0.51
1:F:39:LEU:O	1:F:89:PHE:HA	2.10	0.51
1:A:50:LEU:O	1:A:182:ALA:HA	2.09	0.51
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.32	0.50
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.46	0.50
2:R:359:HIS:O	2:R:366:ASN:HB3	2.12	0.50
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.41	0.50
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.93	0.50
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.46	0.50
1:C:131:PHE:O	1:C:132:ALA:HB2	2.12	0.50
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.94	0.50
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.94	0.50
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.94	0.50
1:A:15:PRO:HB3	1:A:133:ARG:HD2	1.93	0.50
2:O:390:LYS:CD	6:O:649:HOH:O	2.60	0.50
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.47	0.50
1:F:176:GLU:HG3	1:F:180:LYS:N	2.27	0.50
2:O:364:LEU:CD2	2:O:440:ARG:HD3	2.33	0.50
1:F:78:GLU:HB3	1:F:80:GLN:HE21	1.74	0.50
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.93	0.50
1:D:100:ASP:CG	1:D:101:ALA:H	2.16	0.49
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.78	0.49
1:B:78:GLU:HG2	2:N:301:PRO:CG	2.43	0.49
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.12	0.49
1:F:78:GLU:HB3	1:F:80:GLN:NE2	2.27	0.49
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.27	0.49
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.27	0.49
2:Q:453:PRO:HB2	2:R:310:ILE:CD1	2.39	0.49
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.77	0.49
1:B:176:GLU:HA	1:B:180:LYS:O	2.12	0.49
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.42	0.49
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.48	0.49
2:P:451:ASN:HB3	2:P:455:ASP:OD2	2.12	0.49
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.13	0.49
2:R:497:ASN:ND2	2:R:499:GLU:N	2.52	0.49
1:A:162:GLU:OE2	1:C:133:ARG:NH2	2.42	0.48
1:C:143:LEU:HD23	1:C:143:LEU:C	2.34	0.48
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.13	0.48
2:M:405:GLY:HA3	6:M:641:HOH:O	2.12	0.48
2:O:326:THR:HG22	2:O:330:ARG:HD2	1.95	0.48
2:O:359:HIS:O	2:O:366:ASN:HB3	2.14	0.48
2:P:350:ASN:OD1	2:P:352:SER:HB2	2.13	0.48
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.13	0.48
1:A:78:GLU:CG	2:M:301:PRO:CB	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HG23	1:A:122:MET:CE	2.44	0.48
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.95	0.48
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.95	0.48
1:E:143:LEU:HD23	1:E:143:LEU:C	2.32	0.48
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.61	0.48
1:D:50:LEU:O	1:D:182:ALA:HA	2.13	0.48
1:D:177:VAL:O	1:D:180:LYS:HB3	2.14	0.48
1:A:100:ASP:CG	1:A:101:ALA:H	2.17	0.48
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.13	0.48
2:N:406:GLY:O	2:N:447:TYR:HD1	1.97	0.48
2:R:306:SER:CB	2:R:530:GLN:HE21	2.26	0.48
1:D:99:PHE:CE2	2:P:411:LYS:HD2	2.48	0.48
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.78	0.48
2:N:399:MET:HA	2:N:462:HIS:O	2.14	0.48
1:C:31:ARG:NH1	2:O:428:ARG:HG2	2.28	0.48
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.79	0.48
1:C:78:GLU:HG2	2:O:301:PRO:CB	2.44	0.47
1:E:19:ILE:HD11	2:Q:408:TYR:HD1	1.78	0.47
1:F:100:ASP:CG	1:F:101:ALA:H	2.18	0.47
1:C:98:THR:HB	1:C:100:ASP:OD1	2.14	0.47
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.96	0.47
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.28	0.47
1:D:176:GLU:HA	1:D:180:LYS:O	2.14	0.47
1:A:20:GLY:C	1:A:21:LEU:HD23	2.35	0.47
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.95	0.47
1:D:51:LEU:HD11	1:D:126:ILE:HD12	1.95	0.47
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.96	0.47
1:E:161:ILE:HD13	1:E:196:VAL:HG21	1.96	0.47
1:A:51:LEU:HD11	1:A:126:ILE:HD12	1.96	0.47
1:D:24:GLU:O	1:D:27:GLY:N	2.47	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.14	0.47
2:O:315:TRP:HZ2	2:O:503:GLN:HE21	1.62	0.47
2:Q:416:LEU:C	2:Q:416:LEU:CD2	2.83	0.47
2:R:505:ILE:O	2:R:507:LYS:HE3	2.14	0.47
1:A:133:ARG:NH2	1:B:162:GLU:OE1	2.45	0.47
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.95	0.47
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.79	0.47
1:C:98:THR:OG1	1:C:102:GLY:N	2.48	0.47
1:D:19:ILE:HD11	2:P:408:TYR:HD1	1.80	0.47
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.15	0.47
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.50	0.47
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.78	0.47
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.96	0.47
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.97	0.47
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.49	0.46
2:N:522:ARG:NH1	6:N:673:HOH:O	2.18	0.46
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.97	0.46
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.15	0.46
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.44	0.46
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.51	0.46
1:A:176:GLU:OE2	1:A:179:GLY:CA	2.62	0.46
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.97	0.46
1:E:22:ALA:O	1:E:25:ALA:HB3	2.16	0.46
1:F:131:PHE:O	1:F:132:ALA:HB2	2.15	0.46
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.73	0.46
2:O:376:GLU:O	2:O:442:ILE:HA	2.15	0.46
2:N:328:ILE:HD12	2:O:335:ALA:HB2	1.97	0.46
2:N:373:PRO:HB3	2:N:423:PHE:HB2	1.98	0.46
1:C:19:ILE:CD1	2:O:408:TYR:HD2	2.29	0.46
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.50	0.46
2:O:416:LEU:C	2:O:416:LEU:CD2	2.84	0.46
2:P:318:LYS:HA	2:P:318:LYS:HD3	1.56	0.46
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.51	0.46
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.79	0.46
1:B:143:LEU:C	1:B:143:LEU:HD23	2.36	0.46
2:N:416:LEU:HD23	2:N:416:LEU:C	2.36	0.46
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.62	0.46
1:C:19:ILE:O	2:O:426:VAL:HG21	2.16	0.46
1:F:120:VAL:HA	1:F:121:PRO:HD3	1.81	0.46
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.16	0.45
1:D:51:LEU:CD1	1:D:126:ILE:HD12	2.46	0.45
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.80	0.45
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.51	0.45
1:F:78:GLU:HG2	2:R:301:PRO:HG2	1.97	0.45
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.84	0.45
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.98	0.45
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.45
1:D:61:HIS:ND1	1:E:163:GLN:HG3	2.32	0.45
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.98	0.45
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.75	0.45
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:OE2	1:B:94:ARG:HD3	2.16	0.45
1:C:52:LEU:C	1:C:52:LEU:HD22	2.37	0.45
1:D:131:PHE:O	1:D:132:ALA:HB2	2.16	0.45
2:Q:522:ARG:NE	2:Q:524:ASP:OD1	2.49	0.45
1:A:176:GLU:HG3	1:A:180:LYS:C	2.36	0.45
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.98	0.45
1:C:98:THR:O	1:C:102:GLY:HA2	2.16	0.45
2:O:403:ASN:HB2	6:O:613:HOH:O	2.17	0.45
2:O:465:ILE:HD12	2:O:465:ILE:N	2.32	0.45
1:E:24:GLU:O	1:E:27:GLY:N	2.47	0.45
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.97	0.45
2:P:359:HIS:O	2:P:366:ASN:HB3	2.16	0.45
2:R:307:ARG:CG	2:R:533:THR:HG22	2.46	0.45
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.77	0.45
2:R:478:LEU:C	2:R:478:LEU:HD23	2.37	0.45
2:O:493:LYS:HB2	2:O:493:LYS:HE3	1.78	0.45
1:D:98:THR:OG1	1:D:102:GLY:N	2.44	0.45
2:R:385:VAL:O	2:R:526:VAL:HA	2.17	0.45
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.99	0.45
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.17	0.45
2:N:478:LEU:C	2:N:478:LEU:HD23	2.37	0.44
2:P:326:THR:CG2	2:P:330:ARG:HD2	2.45	0.44
1:E:174:ARG:HE	1:E:181:THR:HG23	1.82	0.44
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.51	0.44
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.88	0.44
2:P:376:GLU:O	2:P:442:ILE:HA	2.16	0.44
1:D:70:VAL:HG11	1:D:106:LEU:CD2	2.47	0.44
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.43	0.44
2:N:356:PHE:CE2	2:N:428:ARG:HD3	2.53	0.44
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.99	0.44
1:F:146:ASP:OD1	1:F:174:ARG:HB2	2.17	0.44
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.47	0.44
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.47	0.44
1:B:19:ILE:HG21	2:N:410:HIS:HB2	2.00	0.44
1:E:41:LYS:HD2	1:E:87:ASN:O	2.17	0.44
1:E:110:LYS:HG3	1:E:111:PRO:HD2	1.98	0.44
1:F:32:ASP:HB2	6:F:1362:HOH:O	2.17	0.44
2:N:486:ILE:HB	2:N:487:PRO:HD3	2.00	0.44
5:M:550:DHB:O2	6:M:731:HOH:O	2.20	0.44
2:O:400:TRP:HA	2:O:425:GLY:O	2.18	0.44
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:465:ILE:HD12	2:Q:465:ILE:N	2.33	0.44
1:F:176:GLU:HG3	1:F:180:LYS:H	1.83	0.44
2:R:356:PHE:HD1	2:R:428:ARG:HD3	1.82	0.44
2:R:416:LEU:C	2:R:416:LEU:CD2	2.85	0.44
1:A:19:ILE:O	2:M:426:VAL:HG21	2.18	0.43
2:M:350:ASN:OD1	2:M:352:SER:N	2.36	0.43
2:Q:522:ARG:NH2	2:Q:524:ASP:OD1	2.51	0.43
2:M:416:LEU:C	2:M:416:LEU:CD2	2.87	0.43
1:C:4:LEU:HB3	2:O:387:GLN:HB3	1.99	0.43
1:D:114:VAL:HG23	1:D:122:MET:CE	2.48	0.43
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.84	0.43
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.83	0.43
1:E:73:ALA:HB1	1:E:78:GLU:N	2.33	0.43
2:M:453:PRO:O	2:P:515:PRO:HB3	2.17	0.43
1:D:168:GLU:HA	1:D:171:ILE:HD12	2.00	0.43
1:E:94:ARG:NH2	2:Q:398:GLU:OE2	2.44	0.43
1:A:98:THR:O	1:A:102:GLY:HA2	2.18	0.43
1:B:78:GLU:HG2	2:N:301:PRO:CB	2.48	0.43
2:P:313:ARG:O	2:P:318:LYS:CE	2.64	0.43
2:P:416:LEU:CD2	2:P:416:LEU:C	2.87	0.43
1:F:16:TYR:O	1:F:19:ILE:HG23	2.19	0.43
2:R:383:ARG:NH2	2:R:391:PRO:HG3	2.34	0.43
1:E:50:LEU:O	1:E:182:ALA:HA	2.19	0.43
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.99	0.43
1:E:8:THR:HA	1:E:9:PRO:HD3	1.86	0.43
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.84	0.43
2:M:359:HIS:O	2:M:366:ASN:HB3	2.19	0.43
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.77	0.43
2:Q:306:SER:O	2:Q:307:ARG:NH1	2.51	0.43
1:F:8:THR:HA	1:F:9:PRO:HD3	1.85	0.43
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.19	0.42
2:Q:405:GLY:HA3	6:Q:1008:HOH:O	2.18	0.42
2:Q:411:LYS:HB3	2:Q:411:LYS:HE2	1.68	0.42
1:F:15:PRO:HB3	1:F:133:ARG:HD2	2.01	0.42
2:M:497:ASN:HD22	2:M:499:GLU:N	2.14	0.42
2:N:416:LEU:C	2:N:416:LEU:CD2	2.87	0.42
2:O:373:PRO:HB3	2:O:423:PHE:HB2	2.01	0.42
1:D:18:HIS:CE1	1:D:99:PHE:CE1	3.08	0.42
1:F:81:ASP:OD1	1:F:81:ASP:N	2.49	0.42
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.68	0.42
2:P:497:ASN:HD22	2:P:497:ASN:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:O	1:B:180:LYS:HB3	2.19	0.42
1:E:19:ILE:O	2:Q:426:VAL:HG21	2.19	0.42
2:M:400:TRP:HA	2:M:425:GLY:O	2.19	0.42
2:N:383:ARG:HA	2:N:435:GLY:O	2.19	0.42
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	2.01	0.42
2:R:331:SER:HA	2:R:332:PRO:HD3	1.92	0.42
2:M:406:GLY:O	2:M:447:TYR:HD1	2.00	0.42
1:D:52:LEU:C	1:D:52:LEU:HD22	2.40	0.42
2:P:497:ASN:HD21	2:P:499:GLU:HB2	1.85	0.42
2:R:449:TRP:CD1	2:R:449:TRP:N	2.87	0.42
2:M:318:LYS:HD3	2:M:318:LYS:HA	1.83	0.42
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.75	0.42
2:N:497:ASN:HD22	2:N:497:ASN:C	2.21	0.42
2:P:522:ARG:NH1	6:P:670:HOH:O	2.52	0.42
1:E:52:LEU:HA	1:E:104:TRP:O	2.20	0.42
1:E:176:GLU:HG3	1:E:180:LYS:O	2.19	0.42
1:B:174:ARG:HE	1:B:181:THR:HG23	1.84	0.42
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.83	0.42
2:O:381:ALA:O	2:O:522:ARG:HA	2.20	0.42
2:P:420:ASP:HA	2:P:421:PRO:HD2	1.92	0.42
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.17	0.42
2:N:326:THR:HG22	2:N:330:ARG:HD2	2.00	0.42
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.55	0.42
2:R:495:ILE:CG2	2:R:500:ALA:HB3	2.50	0.42
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.82	0.42
1:B:176:GLU:OE2	1:B:179:GLY:C	2.59	0.41
1:C:176:GLU:HG3	1:C:180:LYS:C	2.40	0.41
1:F:131:PHE:CD2	1:F:138:HIS:HB3	2.55	0.41
1:C:100:ASP:CG	1:C:101:ALA:H	2.23	0.41
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.85	0.41
2:Q:356:PHE:HZ	2:Q:430:LEU:HD13	1.84	0.41
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.20	0.41
1:F:143:LEU:HD23	1:F:144:TYR:N	2.35	0.41
2:M:478:LEU:HD23	2:M:478:LEU:C	2.40	0.41
1:B:52:LEU:HA	1:B:104:TRP:O	2.20	0.41
2:O:308:PHE:CE2	2:O:530:GLN:HB2	2.55	0.41
1:F:100:ASP:OD1	1:F:100:ASP:N	2.48	0.41
1:F:188:ARG:HG3	1:F:188:ARG:HH11	1.85	0.41
2:M:409:ARG:NH2	2:M:420:ASP:O	2.52	0.41
1:E:44:ALA:O	1:E:48:HIS:NE2	2.36	0.41
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.78	0.41
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.99	0.41
1:D:52:LEU:HA	1:D:104:TRP:O	2.20	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.92	0.41
1:A:165:GLN:NE2	1:A:165:GLN:H	2.18	0.41
1:C:99:PHE:CE2	2:O:411:LYS:HD3	2.54	0.41
2:P:326:THR:HG22	2:P:326:THR:O	2.21	0.41
1:E:19:ILE:HG21	2:Q:410:HIS:HB2	2.03	0.41
2:R:522:ARG:NH1	6:R:1272:HOH:O	2.53	0.41
1:B:20:GLY:HA2	2:N:426:VAL:HG13	2.02	0.41
1:C:28:ASN:HB3	1:C:29:PRO:HD2	2.02	0.41
1:C:74:ASP:C	1:C:74:ASP:OD1	2.59	0.41
1:E:165:GLN:N	1:E:165:GLN:NE2	2.21	0.41
1:A:99:PHE:HE2	2:M:411:LYS:HD3	1.86	0.41
1:C:140:HIS:O	1:C:197:PHE:HA	2.21	0.41
2:O:484:PRO:O	2:O:487:PRO:HD2	2.20	0.41
2:Q:487:PRO:HG2	6:Q:1078:HOH:O	2.21	0.41
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.67	0.41
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.68	0.41
2:P:372:LEU:HA	2:P:373:PRO:HD3	1.77	0.41
2:P:406:GLY:O	2:P:447:TYR:HD1	2.04	0.41
2:P:483:ASP:HA	2:P:484:PRO:HD2	1.94	0.41
1:F:49:ILE:HA	1:F:180:LYS:HE3	2.03	0.41
2:M:448:PRO:HB2	2:P:516:MET:HA	2.03	0.41
1:B:163:GLN:HA	1:B:164:PRO:HD3	1.94	0.41
2:N:364:LEU:HD11	2:N:442:ILE:HG23	2.02	0.41
5:O:550:DHB:H6	6:O:746:HOH:O	2.21	0.41
1:D:18:HIS:CE1	1:D:99:PHE:HE1	2.38	0.41
1:F:38:ARG:HA	1:F:107:HIS:HB2	2.03	0.41
1:B:4:LEU:HB3	2:N:387:GLN:HB3	2.03	0.40
2:O:390:LYS:HA	2:O:391:PRO:HD3	1.91	0.40
1:E:19:ILE:O	2:Q:426:VAL:CG2	2.69	0.40
2:R:376:GLU:O	2:R:442:ILE:HA	2.21	0.40
2:N:386:ASP:HA	2:N:527:LEU:O	2.22	0.40
2:O:356:PHE:HE1	2:O:428:ARG:HD3	1.85	0.40
1:D:31:ARG:NH1	2:P:428:ARG:HG2	2.36	0.40
1:F:154:LYS:HD2	1:F:154:LYS:HA	1.79	0.40
1:A:19:ILE:HG21	1:A:19:ILE:HD13	1.70	0.40
1:A:180:LYS:HG2	1:A:181:THR:N	2.36	0.40
1:C:158:LEU:HD12	1:C:158:LEU:HA	1.87	0.40
2:Q:356:PHE:CZ	2:Q:430:LEU:HD13	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG22	1:A:26:ALA:HB1	2.03	0.40
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.52	0.40
1:B:5:LEU:HA	1:B:6:PRO:HD3	1.90	0.40
2:N:395:THR:O	2:N:430:LEU:HA	2.22	0.40
2:O:416:LEU:C	2:O:416:LEU:HD23	2.40	0.40
2:M:316:HIS:HB3	2:M:317:PRO:HD2	2.02	0.40
2:P:431:THR:HG22	2:P:437:TYR:HB3	2.03	0.40
1:E:36:TRP:CE3	1:E:36:TRP:HA	2.56	0.40
2:Q:438:SER:O	4:Q:601:BME:H22	2.21	0.40
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.51	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%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	F	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	R	229/238 (96%)	220 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2562/2628 (98%)	2475 (97%)	87 (3%)	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%)	155 (96%)	7 (4%)	29	36
1	B	162/163 (99%)	154 (95%)	8 (5%)	25	31
1	C	162/163 (99%)	157 (97%)	5 (3%)	40	51
1	D	162/163 (99%)	155 (96%)	7 (4%)	29	36
1	E	162/163 (99%)	156 (96%)	6 (4%)	34	43
1	F	162/163 (99%)	157 (97%)	5 (3%)	40	51
2	M	196/202 (97%)	186 (95%)	10 (5%)	24	29
2	N	196/202 (97%)	186 (95%)	10 (5%)	24	29
2	O	196/202 (97%)	184 (94%)	12 (6%)	18	21
2	P	196/202 (97%)	184 (94%)	12 (6%)	18	21
2	Q	196/202 (97%)	188 (96%)	8 (4%)	30	39
2	R	196/202 (97%)	185 (94%)	11 (6%)	21	25
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	26	33

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	52	LEU
1	A	158	LEU
1	A	164	PRO

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Mol	Chain	Res	Type
1	A	165	GLN
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	399	MET
2	M	416	LEU
2	M	428	ARG
2	M	468	PRO
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	165	GLN
1	B	176	GLU
1	B	184	ARG
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	433	SER
2	N	440	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	165	GLN
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	399	MET
2	O	411	LYS
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP

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Mol	Chain	Res	Type
2	O	440	ARG
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	52	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	372	LEU
2	P	391	PRO
2	P	395	THR
2	P	399	MET
2	P	411	LYS
2	P	416	LEU
2	P	428	ARG
2	P	440	ARG
2	P	478	LEU
2	P	497	ASN
2	P	534	HIS
1	E	19	ILE
1	E	38	ARG
1	E	52	LEU
1	E	66	SER
1	E	165	GLN
1	E	180	LYS
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
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	165	GLN
1	F	181	THR

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Mol	Chain	Res	Type
2	R	372	LEU
2	R	395	THR
2	R	399	MET
2	R	416	LEU
2	R	428	ARG
2	R	434	ASP
2	R	440	ARG
2	R	478	LEU
2	R	497	ASN
2	R	507	LYS
2	R	534	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	497	ASN
2	N	503	GLN
1	C	18	HIS
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	18	HIS
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN

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Mol	Chain	Res	Type
1	F	165	GLN
2	R	361	HIS
2	R	422	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	DHB	N	602	-	11,11,11	1.08	0	15,15,15	1.21	2 (13%)
4	BME	M	601	2	3,3,3	0.21	0	1,2,2	0.10	0
5	DHB	O	550	3	11,11,11	1.51	4 (36%)	15,15,15	1.30	2 (13%)
5	DHB	N	551	-	11,11,11	1.19	0	15,15,15	1.15	2 (13%)
5	DHB	N	550	3	11,11,11	1.37	3 (27%)	15,15,15	1.33	2 (13%)
5	DHB	P	551	-	11,11,11	1.26	0	15,15,15	1.33	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DHB	P	550	3	11,11,11	1.33	1 (9%)	15,15,15	1.29	2 (13%)
5	DHB	Q	550	3	11,11,11	1.44	2 (18%)	15,15,15	1.15	2 (13%)
5	DHB	M	550	3	11,11,11	1.29	1 (9%)	15,15,15	1.18	2 (13%)
4	BME	N	601	2	3,3,3	0.18	0	1,2,2	0.30	0
5	DHB	Q	551	-	11,11,11	1.25	0	15,15,15	1.27	2 (13%)
5	DHB	R	550	3	11,11,11	1.39	3 (27%)	15,15,15	1.23	2 (13%)
5	DHB	R	551	-	11,11,11	1.20	1 (9%)	15,15,15	1.22	2 (13%)
4	BME	P	601	2	3,3,3	0.40	0	1,2,2	0.75	0
4	BME	R	601	2	3,3,3	0.65	0	1,2,2	0.82	0
4	BME	O	601	2	3,3,3	0.56	0	1,2,2	0.42	0
4	BME	Q	601	2	3,3,3	0.35	0	1,2,2	0.24	0
5	DHB	M	551	-	11,11,11	1.15	0	15,15,15	1.41	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DHB	N	602	-	-	0/4/4/4	0/1/1/1
4	BME	M	601	2	-	1/1/1/1	-
5	DHB	O	550	3	-	0/4/4/4	0/1/1/1
5	DHB	N	551	-	-	0/4/4/4	0/1/1/1
5	DHB	N	550	3	-	0/4/4/4	0/1/1/1
5	DHB	P	551	-	-	0/4/4/4	0/1/1/1
5	DHB	P	550	3	-	0/4/4/4	0/1/1/1
5	DHB	Q	550	3	-	0/4/4/4	0/1/1/1
5	DHB	M	550	3	-	0/4/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	-
5	DHB	Q	551	-	-	0/4/4/4	0/1/1/1
5	DHB	R	550	3	-	0/4/4/4	0/1/1/1
5	DHB	R	551	-	-	0/4/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-
4	BME	R	601	2	-	0/1/1/1	-
4	BME	O	601	2	-	0/1/1/1	-
4	BME	Q	601	2	-	0/1/1/1	-
5	DHB	M	551	-	-	0/4/4/4	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	DHB	O4-C4	3.03	1.42	1.36
5	Q	550	DHB	C2-C1	2.66	1.43	1.39
5	O	550	DHB	O4-C4	2.63	1.41	1.36
5	O	550	DHB	C6-C1	2.54	1.43	1.39
5	N	550	DHB	O4-C4	2.34	1.41	1.36
5	N	550	DHB	C2-C3	2.26	1.42	1.38
5	R	550	DHB	C2-C1	2.24	1.42	1.39
5	M	550	DHB	C6-C1	2.20	1.43	1.39
5	R	550	DHB	O2-C	-2.11	1.24	1.30
5	R	551	DHB	O3-C3	2.10	1.40	1.36
5	N	550	DHB	C6-C1	2.10	1.42	1.39
5	Q	550	DHB	O4-C4	2.10	1.40	1.36
5	O	550	DHB	O2-C	-2.09	1.24	1.30
5	R	550	DHB	C6-C1	2.07	1.42	1.39
5	O	550	DHB	C2-C1	2.04	1.42	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	550	DHB	O2-C-O1	-3.51	115.55	123.35
5	R	550	DHB	O2-C-O1	-3.24	116.15	123.35
5	P	550	DHB	O2-C-O1	-3.09	116.49	123.35
5	O	550	DHB	O2-C-C1	3.04	122.75	114.85
5	M	551	DHB	O2-C-C1	2.98	122.59	114.85
5	M	551	DHB	O2-C-O1	-2.97	116.75	123.35
5	O	550	DHB	O2-C-O1	-2.88	116.96	123.35
5	P	551	DHB	O2-C-O1	-2.83	117.06	123.35
5	P	551	DHB	O2-C-C1	2.83	122.18	114.85
5	Q	551	DHB	O2-C-C1	2.69	121.82	114.85
5	N	551	DHB	O2-C-C1	2.67	121.77	114.85
5	M	550	DHB	O2-C-C1	2.67	121.77	114.85
5	Q	551	DHB	O2-C-O1	-2.60	117.58	123.35
5	N	550	DHB	O2-C-C1	2.59	121.56	114.85
5	P	550	DHB	O2-C-C1	2.59	121.56	114.85
5	N	551	DHB	O2-C-O1	-2.41	117.99	123.35
5	N	602	DHB	O2-C-O1	-2.41	118.00	123.35
5	R	550	DHB	O2-C-C1	2.35	120.94	114.85
5	N	602	DHB	O2-C-C1	2.34	120.91	114.85
5	Q	550	DHB	O2-C-O1	-2.22	118.43	123.35
5	M	551	DHB	C6-C5-C4	-2.20	118.25	120.50
5	M	550	DHB	O2-C-O1	-2.19	118.49	123.35
5	Q	550	DHB	O2-C-C1	2.18	120.50	114.85
5	R	551	DHB	O2-C-C1	2.06	120.19	114.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	551	DHB	C6-C5-C4	-2.02	118.43	120.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	550	DHB	1	0
5	M	550	DHB	1	0
4	Q	601	BME	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.