



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:27 AM UTC

PDB ID : 3PCA / pdb_00003pca
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

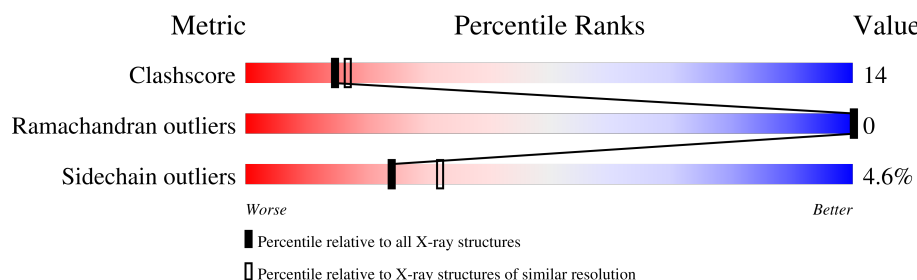
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	71% 24% .
1	B	200	72% 22% 6% .
1	C	200	66% 26% 6% .
1	D	200	69% 24% 6% .
1	E	200	60% 34% 5% .
1	F	200	64% 30% 6%
2	M	238	68% 24% 5% .
2	N	238	69% 25% . . .

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Mol	Chain	Length	Quality of chain
2	O	238	68%26% ...
2	P	238	70%21%6% .
2	Q	238	70%22%5% .
2	R	238	64%30% ..

2 Entry composition

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
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			

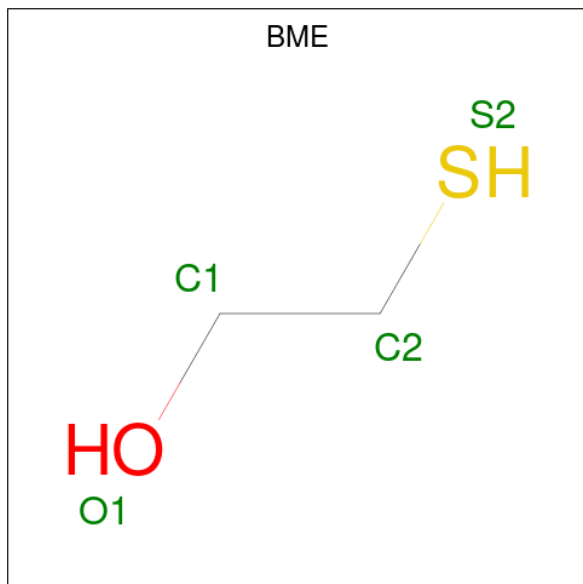
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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 (CCD ID: FE) (formula: Fe).

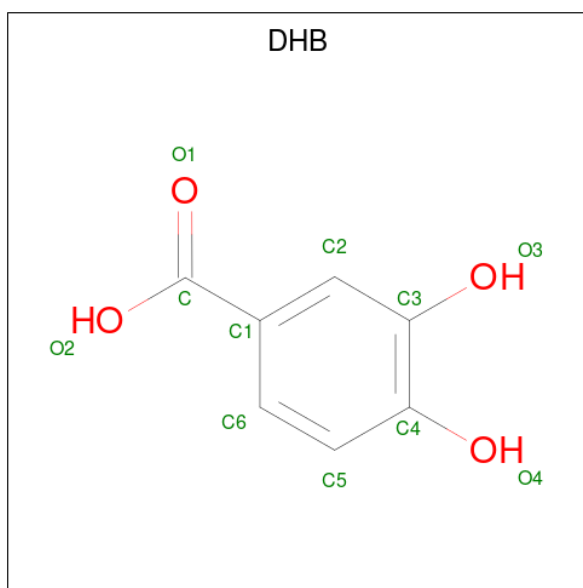
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: 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

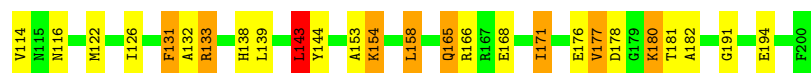
- Molecule 5 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: $C_7H_6O_4$).



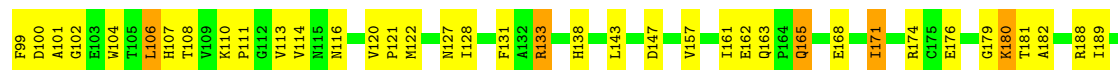
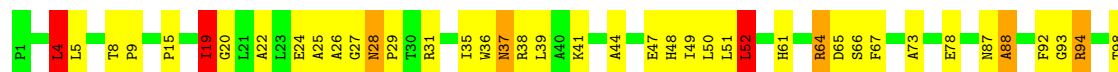
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	C	O	0	0
			11	7	4		
5	M	1	Total	C	O	0	0
			11	7	4		
5	N	1	Total	C	O	0	0
			11	7	4		
5	N	1	Total	C	O	0	0
			11	7	4		
5	N	1	Total	C	O	0	0
			11	7	4		
5	O	1	Total	C	O	0	0
			11	7	4		
5	P	1	Total	C	O	0	0
			11	7	4		
5	P	1	Total	C	O	0	0
			11	7	4		
5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

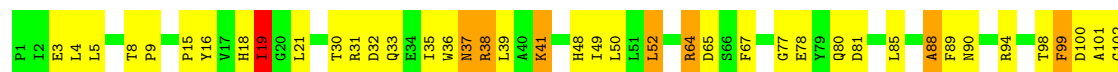
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	84	Total 84	O 84	0	0
6	M	148	Total 148	O 148	0	0
6	B	78	Total 78	O 78	0	0
6	N	160	Total 160	O 160	0	0
6	C	83	Total 83	O 83	0	0
6	O	146	Total 146	O 146	0	0
6	D	76	Total 76	O 76	0	0
6	P	149	Total 149	O 149	0	0
6	E	79	Total 79	O 79	0	0
6	Q	156	Total 156	O 156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



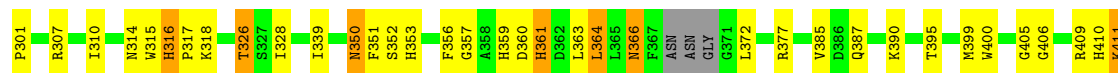
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

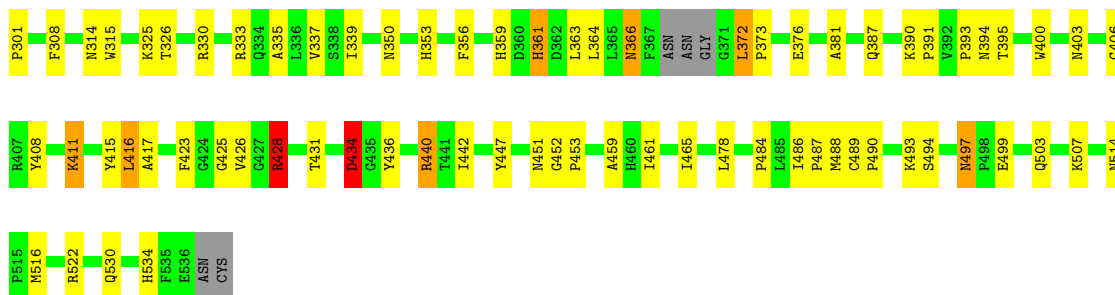


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



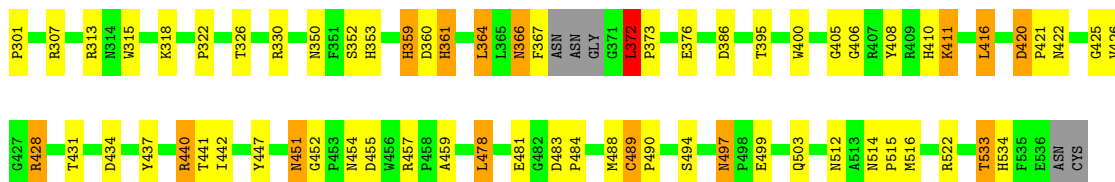
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain 0: 68% 26% ...



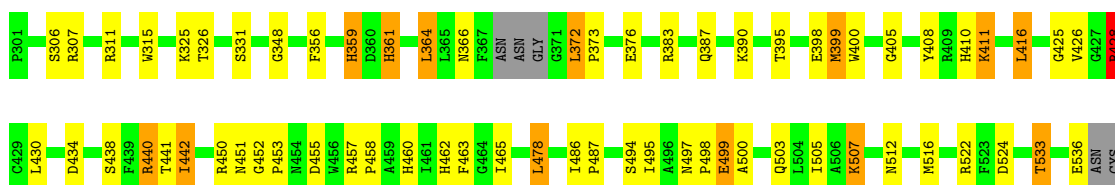
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 70% 21% 6%



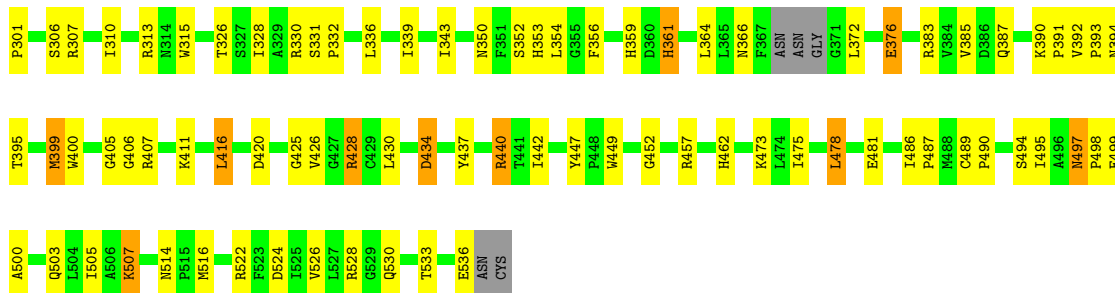
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 70% 22% 5%



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 64% 30% . .



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	196.30Å 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

5.1 Standard geometry

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	1.15	2/1611 (0.1%)	1.75	23/2195 (1.0%)
1	B	1.15	2/1611 (0.1%)	1.72	19/2195 (0.9%)
1	C	1.17	0/1611	1.72	27/2195 (1.2%)
1	D	1.18	2/1611 (0.1%)	1.71	30/2195 (1.4%)
1	E	1.20	1/1611 (0.1%)	1.73	25/2195 (1.1%)
1	F	1.21	2/1611 (0.1%)	1.75	22/2195 (1.0%)
2	M	1.24	2/1895 (0.1%)	1.77	27/2580 (1.0%)
2	N	1.21	2/1895 (0.1%)	1.74	24/2580 (0.9%)
2	O	1.21	2/1895 (0.1%)	1.76	24/2580 (0.9%)
2	P	1.22	1/1895 (0.1%)	1.74	25/2580 (1.0%)
2	Q	1.25	2/1895 (0.1%)	1.74	25/2580 (1.0%)
2	R	1.23	1/1895 (0.1%)	1.75	28/2580 (1.1%)
All	All	1.20	19/21036 (0.1%)	1.74	299/28650 (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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	451	ASN	CA-C	8.16	1.56	1.52
1	D	94	ARG	CD-NE	-7.71	1.35	1.46
2	N	441	THR	CA-CB	6.77	1.62	1.53
2	Q	441	THR	CA-CB	6.46	1.62	1.54
2	M	451	ASN	CA-C	6.34	1.55	1.52
1	E	108	THR	CA-CB	5.89	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	441	THR	CA-CB	5.79	1.61	1.53
1	A	94	ARG	CD-NE	-5.77	1.38	1.46
2	R	452	GLY	N-CA	5.63	1.52	1.44
2	N	428	ARG	CD-NE	-5.60	1.38	1.46
2	Q	452	GLY	N-CA	5.54	1.52	1.44
1	A	108	THR	CA-CB	5.44	1.61	1.54
1	D	108	THR	CA-CB	5.33	1.61	1.54
2	M	452	GLY	N-CA	5.20	1.52	1.44
1	F	135	ILE	CA-CB	5.15	1.60	1.53
1	B	94	ARG	CD-NE	-5.15	1.39	1.46
1	B	5	LEU	CA-C	5.06	1.59	1.53
1	F	38	ARG	N-CA	5.05	1.53	1.46
2	O	452	GLY	CA-C	5.02	1.58	1.51

All (299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	353	HIS	CA-CB-CG	-11.52	102.28	113.80
2	N	522	ARG	CD-NE-CZ	10.79	139.51	124.40
2	Q	452	GLY	N-CA-C	-10.72	99.25	112.23
1	A	94	ARG	CD-NE-CZ	10.24	138.73	124.40
1	D	94	ARG	CD-NE-CZ	10.24	138.73	124.40
1	B	176	GLU	CB-CG-CD	10.07	129.71	112.60
1	C	94	ARG	CD-NE-CZ	9.81	138.13	124.40
1	E	37	ASN	N-CA-C	9.78	124.46	113.21
2	P	452	GLY	N-CA-C	-9.67	100.53	112.23
2	R	361	HIS	CA-CB-CG	-9.62	104.18	113.80
1	D	94	ARG	CG-CD-NE	9.62	133.15	112.00
2	M	452	GLY	N-CA-C	-9.61	100.29	112.10
2	P	457	ARG	CD-NE-CZ	9.60	137.84	124.40
2	O	452	GLY	N-CA-C	-9.39	100.55	112.10
1	C	94	ARG	NE-CZ-NH2	-9.30	110.83	119.20
2	N	452	GLY	N-CA-C	-9.20	100.78	112.10
1	F	37	ASN	N-CA-C	9.15	123.17	112.93
2	R	440	ARG	NE-CZ-NH2	-9.07	111.04	119.20
1	D	37	ASN	N-CA-C	9.04	123.06	112.93
2	P	359	HIS	CA-CB-CG	-8.78	105.02	113.80
1	A	37	ASN	N-CA-C	8.70	122.68	112.93
2	P	440	ARG	NE-CZ-NH2	-8.57	111.49	119.20
2	N	440	ARG	NE-CZ-NH2	-8.41	111.63	119.20
2	M	353	HIS	CA-CB-CG	-8.39	105.41	113.80
2	R	353	HIS	CA-CB-CG	-8.22	105.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	361	HIS	CA-CB-CG	-8.21	105.59	113.80
1	A	94	ARG	CB-CG-CD	8.21	130.19	111.30
2	Q	440	ARG	NE-CZ-NH2	-8.21	111.81	119.20
2	M	440	ARG	NE-CZ-NH2	-8.15	111.86	119.20
1	B	37	ASN	N-CA-C	8.14	122.79	113.02
1	D	94	ARG	CB-CG-CD	8.06	129.85	111.30
2	R	434	ASP	CA-CB-CG	-7.89	104.71	112.60
1	D	19	ILE	CB-CA-C	7.69	122.11	112.04
1	D	94	ARG	NE-CZ-NH2	-7.58	112.38	119.20
1	C	37	ASN	N-CA-C	7.54	121.37	112.93
2	O	361	HIS	CA-CB-CG	-7.40	106.40	113.80
1	A	21	LEU	N-CA-C	7.37	123.17	113.30
2	O	451	ASN	O-C-N	7.29	126.22	120.83
2	M	457	ARG	CD-NE-CZ	7.26	134.57	124.40
2	O	339	ILE	O-C-N	7.24	126.25	121.69
1	C	94	ARG	NE-CZ-NH1	7.23	128.73	121.50
1	C	19	ILE	CA-CB-CG1	7.22	122.68	110.40
1	E	52	LEU	CB-CA-C	7.21	125.95	110.45
1	D	94	ARG	NE-CZ-NH1	7.20	128.69	121.50
1	C	19	ILE	CB-CA-C	7.18	122.54	112.05
1	A	5	LEU	N-CA-C	-7.13	100.77	109.83
2	R	420	ASP	CB-CA-C	7.05	118.26	110.15
2	P	353	HIS	CA-CB-CG	-7.00	106.80	113.80
2	P	361	HIS	CA-CB-CG	-6.98	106.82	113.80
2	O	514	ASN	CA-CB-CG	6.95	119.55	112.60
2	M	494	SER	N-CA-C	-6.87	103.81	111.71
1	A	23	LEU	CB-CA-C	6.83	122.18	110.84
1	A	87	ASN	CA-CB-CG	6.82	119.42	112.60
2	P	512	ASN	CA-CB-CG	-6.82	105.78	112.60
2	M	428	ARG	CB-CG-CD	6.73	126.79	111.30
2	Q	434	ASP	CA-CB-CG	-6.73	105.87	112.60
1	D	28	ASN	O-C-N	6.71	126.78	121.55
1	C	100	ASP	CA-CB-CG	-6.70	105.90	112.60
1	C	47	GLU	CB-CG-CD	6.62	123.85	112.60
1	F	5	LEU	N-CA-C	-6.60	101.45	109.83
2	M	339	ILE	O-C-N	6.57	125.83	121.69
2	Q	460	HIS	CA-CB-CG	-6.57	107.23	113.80
2	Q	457	ARG	CD-NE-CZ	6.49	133.49	124.40
2	Q	512	ASN	CA-CB-CG	-6.47	106.13	112.60
2	O	440	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	E	157	VAL	CB-CA-C	6.47	120.51	112.04
1	E	171	ILE	N-CA-CB	-6.46	103.66	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	366	ASN	N-CA-C	6.45	121.01	113.20
2	O	314	ASN	CB-CA-C	6.45	120.87	109.65
1	E	5	LEU	N-CA-C	-6.42	101.22	110.08
2	N	533	THR	CA-CB-OG1	-6.40	100.00	109.60
2	Q	499	GLU	CB-CG-CD	6.38	123.45	112.60
2	Q	499	GLU	CA-CB-CG	6.38	126.85	114.10
2	R	393	PRO	CA-C-N	6.36	131.40	122.36
2	R	393	PRO	C-N-CA	6.36	131.40	122.36
1	A	171	ILE	N-CA-C	6.34	116.95	107.51
2	M	326	THR	CA-CB-OG1	-6.33	100.11	109.60
2	O	434	ASP	CA-CB-CG	-6.33	106.28	112.60
2	Q	533	THR	CA-CB-OG1	-6.32	100.11	109.60
2	N	442	ILE	CA-CB-CG2	6.32	121.24	110.50
2	M	361	HIS	CA-CB-CG	-6.31	107.49	113.80
2	R	457	ARG	CA-CB-CG	6.30	126.70	114.10
2	P	533	THR	CA-CB-OG1	-6.29	100.17	109.60
1	B	177	VAL	CB-CA-C	6.29	118.21	110.73
1	C	99	PHE	CA-CB-CG	6.28	120.08	113.80
1	C	5	LEU	N-CA-C	-6.27	101.87	109.83
1	A	94	ARG	CG-CD-NE	6.27	125.79	112.00
1	D	23	LEU	CB-CA-C	6.24	121.20	110.84
2	P	451	ASN	O-C-N	6.22	125.43	120.83
2	N	428	ARG	CG-CD-NE	6.19	125.61	112.00
2	O	366	ASN	N-CA-C	6.19	120.69	113.20
2	M	481	GLU	CB-CG-CD	6.18	123.11	112.60
2	Q	450	ARG	CD-NE-CZ	-6.18	115.75	124.40
1	B	5	LEU	N-CA-C	-6.17	101.57	110.08
1	F	90	ASN	CA-CB-CG	6.16	118.76	112.60
1	C	125	HIS	CA-CB-CG	-6.15	107.65	113.80
2	R	452	GLY	N-CA-C	-6.12	99.84	112.34
1	B	94	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	D	5	LEU	N-CA-C	-6.09	102.09	109.83
1	C	41	LYS	N-CA-C	-6.09	101.89	110.29
1	E	64	ARG	CD-NE-CZ	-6.07	115.90	124.40
1	C	32	ASP	CA-CB-CG	6.03	118.63	112.60
1	F	150	GLN	O-C-N	6.02	128.29	122.03
2	R	494	SER	N-CA-C	-6.01	105.21	112.54
1	D	18	HIS	CA-CB-CG	-6.00	107.80	113.80
2	R	514	ASN	O-C-N	6.00	126.83	121.19
1	F	133	ARG	N-CA-C	-5.99	101.80	110.24
2	P	434	ASP	CA-CB-CG	-5.96	106.64	112.60
1	E	38	ARG	CD-NE-CZ	-5.95	116.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	171	ILE	N-CA-CB	-5.92	104.01	111.41
1	D	133	ARG	N-CA-CB	-5.91	100.65	109.69
1	F	21	LEU	N-CA-CB	-5.91	102.00	110.80
1	F	38	ARG	CA-CB-CG	5.89	125.88	114.10
1	B	52	LEU	CB-CA-C	5.88	122.47	109.94
1	B	184	ARG	NE-CZ-NH2	-5.87	113.91	119.20
2	N	439	PHE	O-C-N	5.85	130.06	123.27
1	D	43	ASP	CA-CB-CG	-5.85	106.75	112.60
1	D	171	ILE	N-CA-C	5.84	116.52	107.99
1	B	94	ARG	CB-CG-CD	5.83	124.72	111.30
2	N	333	ARG	N-CA-C	-5.83	106.78	114.31
1	E	127	ASN	CA-CB-CG	-5.83	106.78	112.60
1	A	30	THR	CA-CB-OG1	-5.82	100.86	109.60
1	C	52	LEU	CB-CA-C	5.82	122.97	110.45
1	C	38	ARG	CD-NE-CZ	-5.81	116.26	124.40
1	C	18	HIS	CA-CB-CG	-5.81	107.99	113.80
1	F	64	ARG	CD-NE-CZ	-5.80	116.27	124.40
1	D	38	ARG	CD-NE-CZ	-5.80	116.28	124.40
1	F	30	THR	CA-CB-OG1	-5.80	100.91	109.60
1	B	18	HIS	CA-CB-CG	-5.79	108.00	113.80
1	A	19	ILE	CB-CA-C	5.79	121.14	112.16
1	E	28	ASN	O-C-N	5.79	126.07	121.55
1	A	78	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	198	PHE	CA-CB-CG	5.76	119.56	113.80
2	N	353	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	52	LEU	CB-CA-C	5.75	122.80	110.45
2	Q	458	PRO	N-CA-C	-5.74	102.81	111.41
1	A	3	GLU	CB-CG-CD	5.74	122.35	112.60
2	P	420	ASP	CB-CA-C	5.73	116.74	110.15
2	M	314	ASN	N-CA-C	-5.72	106.46	113.50
2	Q	348	GLY	O-C-N	5.72	127.49	121.77
1	B	192	GLU	CA-CB-CG	5.72	125.54	114.10
2	Q	441	THR	N-CA-CB	-5.72	102.39	110.51
2	Q	512	ASN	OD1-CG-ND2	5.72	128.32	122.60
2	M	328	ILE	N-CA-C	5.71	115.84	110.30
2	Q	311	ARG	CD-NE-CZ	5.71	132.39	124.40
2	P	322	PRO	N-CA-C	5.70	122.08	113.81
2	O	350	ASN	CA-CB-CG	-5.70	106.90	112.60
2	R	407	ARG	CD-NE-CZ	-5.70	116.42	124.40
1	A	31	ARG	CD-NE-CZ	5.69	132.37	124.40
1	E	189	ILE	O-C-N	5.68	127.38	121.87
2	N	385	VAL	CA-C-O	-5.67	115.89	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	383	ARG	N-CA-CB	-5.67	101.05	111.37
2	M	460	HIS	CA-CB-CG	-5.67	108.13	113.80
2	N	517	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	100	ASP	CA-CB-CG	-5.65	106.95	112.60
2	O	415	TYR	CB-CA-C	5.65	119.09	109.72
2	Q	442	ILE	CA-CB-CG2	5.64	120.09	110.50
1	E	107	HIS	CA-CB-CG	-5.64	108.16	113.80
1	C	87	ASN	CA-CB-CG	5.64	118.24	112.60
2	Q	325	LYS	N-CA-C	5.63	117.87	111.11
1	D	57	ASP	CA-CB-CG	5.63	118.23	112.60
2	O	428	ARG	CD-NE-CZ	5.62	132.27	124.40
1	D	158	LEU	CB-CA-C	5.60	120.09	110.79
1	D	178	ASP	CA-CB-CG	-5.58	107.02	112.60
2	P	459	ALA	N-CA-C	-5.58	102.13	110.23
1	F	142	ARG	NE-CZ-NH1	5.57	127.07	121.50
2	N	365	LEU	CA-C-O	-5.57	112.58	118.77
1	A	133	ARG	N-CA-C	-5.57	101.81	110.10
2	M	350	ASN	N-CA-CB	5.56	119.28	110.55
1	C	171	ILE	N-CA-C	5.56	115.79	107.51
2	O	337	VAL	CA-C-O	-5.55	114.54	120.59
2	P	512	ASN	OD1-CG-ND2	5.55	128.15	122.60
2	P	481	GLU	CB-CG-CD	5.54	122.03	112.60
1	F	37	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	159	ASN	CA-CB-CG	-5.54	107.06	112.60
1	E	133	ARG	N-CA-CB	-5.54	101.22	109.69
1	B	21	LEU	N-CA-CB	-5.53	102.56	110.80
2	P	386	ASP	CA-CB-CG	5.53	118.13	112.60
2	P	489	CYS	N-CA-C	5.52	117.59	109.42
1	F	19	ILE	CB-CA-C	5.51	120.70	112.16
2	N	378	ILE	CA-C-O	5.51	126.86	121.19
1	F	41	LYS	N-CA-C	-5.50	102.70	110.29
1	C	133	ARG	CA-CB-CG	5.50	125.10	114.10
1	F	99	PHE	CA-CB-CG	5.50	119.30	113.80
2	O	514	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	E	106	LEU	N-CA-CB	-5.49	101.32	111.53
2	M	316	HIS	O-C-N	5.49	127.42	121.60
1	E	99	PHE	CA-CB-CG	5.49	119.29	113.80
2	R	514	ASN	CA-CB-CG	5.48	118.08	112.60
1	C	107	HIS	CA-CB-CG	-5.48	108.32	113.80
2	M	535	PHE	CA-C-O	-5.47	114.24	121.08
2	M	411	LYS	CB-CA-C	-5.47	101.66	110.74
2	N	434	ASP	CA-CB-CG	-5.47	107.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	339	ILE	CB-CA-C	5.46	114.68	109.33
2	N	528	ARG	CA-C-N	5.45	125.15	119.92
2	N	528	ARG	C-N-CA	5.45	125.15	119.92
1	D	133	ARG	NE-CZ-NH2	-5.45	114.30	119.20
2	N	525	ILE	O-C-N	5.45	129.14	123.26
2	R	339	ILE	O-C-N	5.44	125.11	121.69
2	Q	494	SER	N-CA-C	-5.43	105.76	112.38
2	R	376	GLU	O-C-N	5.42	129.69	123.02
2	M	385	VAL	O-C-N	5.42	128.97	123.00
1	C	157	VAL	CB-CA-C	5.42	119.14	112.04
2	O	394	ASN	CA-C-O	-5.42	115.55	121.84
2	Q	359	HIS	CA-CB-CG	-5.42	108.39	113.80
2	M	357	GLY	N-CA-C	-5.41	105.62	112.54
1	C	198	PHE	CA-CB-CG	5.41	119.21	113.80
2	O	417	ALA	N-CA-C	-5.41	102.97	109.83
1	B	4	LEU	N-CA-CB	-5.40	102.22	110.49
1	D	177	VAL	CB-CA-C	5.40	117.71	110.42
1	D	131	PHE	CA-CB-CG	5.39	119.19	113.80
1	F	133	ARG	CA-CB-CG	5.39	124.88	114.10
2	O	333	ARG	N-CA-C	-5.38	107.09	113.97
2	P	367	PHE	CA-C-O	-5.37	111.67	120.80
1	D	171	ILE	N-CA-CB	-5.36	104.94	111.21
1	B	11	GLN	N-CA-CB	5.36	121.50	111.53
1	E	4	LEU	CA-C-O	-5.35	114.92	121.88
1	A	21	LEU	N-CA-CB	-5.34	102.55	110.61
2	N	367	PHE	CA-C-O	-5.34	111.73	120.80
2	O	431	THR	N-CA-CB	5.33	117.88	110.04
1	F	52	LEU	CB-CA-C	5.33	121.92	110.45
2	M	314	ASN	CB-CA-C	5.33	118.99	109.29
1	C	48	HIS	CA-CB-CG	-5.33	108.47	113.80
2	N	514	ASN	O-C-N	5.30	126.17	121.19
2	R	328	ILE	N-CA-C	5.30	115.75	110.23
2	O	325	LYS	N-CA-C	5.29	117.46	111.11
2	M	459	ALA	N-CA-C	-5.29	102.22	110.10
2	N	460	HIS	CA-CB-CG	-5.29	108.51	113.80
1	F	88	ALA	N-CA-C	-5.29	106.33	112.89
2	R	387	GLN	OE1-CD-NE2	5.27	127.87	122.60
1	A	41	LYS	N-CA-C	-5.26	103.03	110.29
1	B	171	ILE	N-CA-C	5.25	115.33	107.51
2	R	430	LEU	CB-CA-C	5.25	118.41	109.75
2	Q	428	ARG	NE-CZ-NH2	-5.25	114.48	119.20
2	N	533	THR	N-CA-C	-5.25	103.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	LEU	CB-CA-C	5.24	118.40	109.75
2	R	336	LEU	N-CA-C	-5.23	103.62	110.53
2	M	496	ALA	N-CA-C	5.23	117.06	111.36
1	B	94	ARG	NE-CZ-NH2	-5.22	114.50	119.20
2	R	457	ARG	CD-NE-CZ	5.22	131.71	124.40
1	C	33	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	R	481	GLU	CB-CG-CD	5.21	121.47	112.60
2	Q	463	PHE	O-C-N	5.21	129.65	123.24
1	D	166	ARG	CA-C-N	5.20	127.25	120.28
1	D	166	ARG	C-N-CA	5.20	127.25	120.28
2	N	483	ASP	O-C-N	5.20	125.83	121.31
1	F	5	LEU	O-C-N	5.20	127.25	121.43
2	M	417	ALA	N-CA-C	-5.19	103.23	109.83
1	D	112	GLY	N-CA-C	-5.19	104.49	112.85
1	B	198	PHE	CA-CB-CG	5.19	118.99	113.80
1	F	140	HIS	CB-CA-C	-5.18	100.75	109.72
1	A	94	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	133	ARG	N-CA-C	-5.17	102.40	110.10
2	O	461	ILE	CA-C-O	-5.17	114.97	120.39
1	C	150	GLN	O-C-N	5.15	127.38	122.07
2	N	459	ALA	N-CA-C	-5.15	102.43	110.10
1	E	47	GLU	CB-CG-CD	5.14	121.35	112.60
1	E	113	VAL	N-CA-CB	-5.14	103.21	110.26
1	D	21	LEU	N-CA-CB	-5.13	103.16	110.80
2	Q	411	LYS	CB-CA-C	-5.13	102.23	110.74
1	C	178	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	133	ARG	CA-CB-CG	5.12	124.33	114.10
1	E	19	ILE	CB-CA-C	5.11	119.52	112.05
1	E	37	ASN	CA-CB-CG	-5.11	107.49	112.60
2	N	361	HIS	CA-CB-CG	-5.11	108.69	113.80
2	R	528	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	E	133	ARG	NE-CZ-NH2	-5.11	114.61	119.20
2	P	366	ASN	N-CA-C	5.10	119.36	113.18
2	Q	331	SER	O-C-N	5.10	126.46	121.66
1	B	183	TYR	N-CA-CB	5.10	119.38	110.81
2	R	313	ARG	CD-NE-CZ	-5.10	117.27	124.40
2	R	394	ASN	CA-CB-CG	-5.09	107.51	112.60
1	E	94	ARG	CG-CD-NE	5.08	123.18	112.00
1	A	137	ILE	CB-CA-C	5.08	118.30	110.28
2	P	422	ASN	CA-CB-CG	-5.07	107.53	112.60
1	F	183	TYR	CA-CB-CG	5.07	123.02	113.90
1	C	5	LEU	O-C-N	5.06	127.10	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	357	GLY	CA-C-N	5.06	127.57	120.28
2	M	357	GLY	C-N-CA	5.06	127.57	120.28
2	P	514	ASN	O-C-N	5.06	125.95	121.19
2	R	354	LEU	CB-CA-C	5.06	118.30	109.65
2	P	494	SER	N-CA-C	-5.05	106.21	112.38
2	P	457	ARG	CA-CB-CG	5.05	124.20	114.10
1	E	162	GLU	N-CA-C	5.04	117.17	111.02
2	R	440	ARG	NH1-CZ-NH2	5.04	125.85	119.30
2	O	494	SER	N-CA-C	-5.04	106.39	112.54
1	D	116	ASN	N-CA-C	-5.03	104.04	110.53
2	P	454	ASN	CA-CB-CG	5.03	117.63	112.60
1	E	133	ARG	N-CA-C	-5.03	102.61	110.10
1	D	143	LEU	CB-CA-C	5.03	118.44	110.19
2	P	372	LEU	CB-CA-C	5.03	115.67	108.68
1	E	128	ILE	O-C-N	5.03	128.48	123.10
2	O	459	ALA	N-CA-C	-5.02	102.62	110.10
1	E	88	ALA	N-CA-C	-5.02	105.90	112.23
1	F	114	VAL	CA-C-O	-5.02	116.40	121.67
2	M	440	ARG	CB-CG-CD	-5.00	99.79	111.30
2	R	376	GLU	CG-CD-OE2	-5.00	106.89	118.40
1	B	106	LEU	N-CA-CB	-5.00	102.17	111.13
2	R	392	VAL	O-C-N	5.00	126.80	121.10

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 ⓘ

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	47	0
1	B	1571	0	1499	47	0
1	C	1571	0	1499	53	0
1	D	1571	0	1499	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1571	0	1499	57	0
1	F	1571	0	1499	67	0
2	M	1840	0	1793	51	0
2	N	1840	0	1793	44	0
2	O	1840	0	1793	51	0
2	P	1840	0	1793	53	0
2	Q	1840	0	1793	54	0
2	R	1840	0	1793	60	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	1	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
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	564	0

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

All (564) 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
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
2:M:508:LEU:HD23	2:P:488:MET:HE1	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:114:VAL:HG23	1:B:122:MET:HE3	1.76	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:F:48:HIS:C	1:F:180:LYS:HZ2	2.04	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
1:C:114:VAL:HG23	1:C:122:MET:HE3	1.78	0.66
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.11	0.66
1:C:78:GLU:HG2	2:O:301:PRO:CG	2.27	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:B:176:GLU:HG3	1:B:180:LYS:C	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.80	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:D:143:LEU:C	1:D:143:LEU:HD23	2.24	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
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.82	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
2:M:497:ASN:HD22	2:M:497:ASN:C	2.09	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.66	0.60
1:A:165:GLN:CD	1:A:165:GLN:H	2.10	0.60
1:C:177:VAL:O	1:C:180:LYS:HB3	2.02	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:F:48:HIS:C	1:F:180:LYS:NZ	2.60	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: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
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.13	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:D:114:VAL:HG23	1:D:122:MET:HE3	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LEU:C	1:F:143:LEU:HD23	2.31	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: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
1:F:176:GLU:OE2	1:F:179:GLY:C	2.49	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:478:LEU:C	2:Q:478:LEU:HD23	2.32	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:C:50:LEU:O	1:C:182:ALA:HA	2.06	0.54
2:R:361:HIS:CD2	2:R:361:HIS:N	2.65	0.54
1:D:100:ASP:CG	1:D:101:ALA:H	2.16	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:E:143:LEU:HD23	1:E:143:LEU:C	2.32	0.53
1:C:143:LEU:HD23	1:C:143:LEU:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.91	0.53
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:A:100:ASP:CG	1:A:101:ALA:H	2.17	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
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.97	0.52
1:F:100:ASP:CG	1:F:101:ALA:H	2.18	0.52
1:A:20:GLY:C	1:A:21:LEU:HD23	2.35	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
2:P:484:PRO:O	2:P:488:MET:HE3	2.10	0.52
2:Q:416:LEU:C	2:Q:416:LEU:CD2	2.83	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:N:416:LEU:HD23	2:N:416:LEU:C	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
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
2:P:400:TRP:HA	2:P:425:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:143:LEU:C	1:B:143:LEU:HD23	2.36	0.50
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.59	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:C:52:LEU:C	1:C:52:LEU:HD22	2.37	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
1:A:176:GLU:HG3	1:A:180:LYS:C	2.36	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
2:O:416:LEU:C	2:O:416:LEU:CD2	2.84	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
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
2:R:478:LEU:C	2:R:478:LEU:HD23	2.37	0.49
1:F:78:GLU:HB3	1:F:80:GLN:NE2	2.27	0.49
2:N:478:LEU:C	2:N:478:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:416:LEU:C	2:R:416:LEU:CD2	2.85	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
1:A:114:VAL:HG23	1:A:122:MET:CE	2.44	0.48
2:M:416:LEU:C	2:M:416:LEU:CD2	2.87	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: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: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
2:P:416:LEU:CD2	2:P:416:LEU:C	2.87	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: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: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:A:114:VAL:CG2	1:A:122:MET:HE3	2.43	0.47
2:N:416:LEU:C	2:N:416:LEU:CD2	2.87	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:P:497:ASN:HD22	2:P:497:ASN:C	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:36:TRP:CG	1:C:37:ASN:H	2.32	0.47
1:D:52:LEU:C	1:D:52:LEU:HD22	2.40	0.47
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.50	0.47
2:N:497:ASN:HD22	2:N:497:ASN:C	2.21	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:B:176:GLU:OE2	1:B:179:GLY:C	2.59	0.46
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.97	0.46
1:C:176:GLU:HG3	1:C:180:LYS:C	2.40	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
1:C:100:ASP:CG	1:C:101:ALA:H	2.23	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: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:C:74:ASP:C	1:C:74:ASP:OD1	2.59	0.46
1:F:3:GLU:OE1	1:F:3:GLU:CA	2.62	0.46
2:M:478:LEU:HD23	2:M:478:LEU:C	2.40	0.46
1:C:19:ILE:O	2:O:426:VAL:HG21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:69:GLU:OE2	1:B:94:ARG:HD3	2.16	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:F:114:VAL:HG23	1:F:122:MET:HE3	1.97	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:O:416:LEU:C	2:O:416:LEU:HD23	2.40	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: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:437:TYR:CD1	2:R:437:TYR:C	2.94	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:P:326:THR:CG2	2:P:330:ARG:HD2	2.45	0.44
1:E:100:ASP:CG	1:E:101:ALA:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:TRP:CG	1:F:37:ASN:H	2.36	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
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
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:O:497:ASN:HD22	2:O:497:ASN:C	2.26	0.43
1:A:143:LEU:C	1:A:143:LEU:HD23	2.43	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
2:P:516:MET:HE3	2:P:516:MET:HB3	1.78	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
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:E:116:ASN:C	1:E:116:ASN:OD1	2.62	0.43
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:176:GLU:OE2	1:A:179:GLY:C	2.62	0.42
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: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:O:484:PRO:O	2:O:488:MET:HE3	2.19	0.42
2:P:478:LEU:C	2:P:478:LEU:HD23	2.43	0.42
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:Q:416:LEU:C	2:Q:416:LEU:HD23	2.44	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:350:ASN:OD1	2:M:350:ASN:C	2.61	0.42
2:M:406:GLY:O	2:M:447:TYR:HD1	2.00	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: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
1:B:165:GLN:H	1:B:165:GLN:CD	2.25	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
1:E:36:TRP:CG	1:E:37:ASN:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:131:PHE:CD2	1:F:138:HIS:HB3	2.55	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:R:416:LEU:C	2:R:416:LEU:HD23	2.45	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
2:N:324:TYR:OH	5:N:550:DHB:O1	2.30	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
1:B:147:ASP:OD2	1:B:183:TYR:OH	2.37	0.41
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
2:O:516:MET:HE3	2:O:516:MET:HB3	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:176:GLU:HG3	1:E:180:LYS:C	2.46	0.41
2:Q:516:MET:HE3	2:Q:516:MET:HB3	1.90	0.41
1:F:38:ARG:HA	1:F:107:HIS:HB2	2.03	0.41
2:R:516:MET:HE3	2:R:516:MET:HB3	1.82	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:R:497:ASN:HD22	2:R:497:ASN:C	2.28	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
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:M:316:HIS:HB3	2:M:317:PRO:HD2	2.02	0.40
2:N:516:MET:HE3	2:N:516:MET:HB3	1.83	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
1:F:110:LYS:NZ	1:F:148:GLU:OE2	2.52	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

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%)	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
All	All	2562/2628 (98%)	2475 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	155 (96%)	7 (4%)	26	35
1	B	162/163 (99%)	153 (94%)	9 (6%)	19	24
1	C	162/163 (99%)	156 (96%)	6 (4%)	30	41
1	D	162/163 (99%)	154 (95%)	8 (5%)	22	29
1	E	162/163 (99%)	155 (96%)	7 (4%)	26	35
1	F	162/163 (99%)	157 (97%)	5 (3%)	35	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	196/202 (97%)	188 (96%)	8 (4%)	27	37
2	N	196/202 (97%)	187 (95%)	9 (5%)	24	32
2	O	196/202 (97%)	185 (94%)	11 (6%)	19	24
2	P	196/202 (97%)	187 (95%)	9 (5%)	24	32
2	Q	196/202 (97%)	188 (96%)	8 (4%)	27	37
2	R	196/202 (97%)	185 (94%)	11 (6%)	19	24
All	All	2148/2190 (98%)	2050 (95%)	98 (5%)	24	32

All (98) 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
1	A	165	GLN
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	478	LEU
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	52	LEU
1	B	143	LEU
1	B	158	LEU
1	B	162	GLU
1	B	165	GLN
1	B	176	GLU
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	416	LEU
2	N	433	SER

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Mol	Chain	Res	Type
2	N	440	ARG
2	N	442	ILE
2	N	497	ASN
2	N	507	LYS
1	C	4	LEU
1	C	19	ILE
1	C	52	LEU
1	C	78	GLU
1	C	94	ARG
1	C	165	GLN
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	411	LYS
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	478	LEU
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	52	LEU
1	D	78	GLU
1	D	143	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	372	LEU
2	P	395	THR
2	P	411	LYS
2	P	416	LEU
2	P	428	ARG
2	P	478	LEU
2	P	497	ASN
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	49	ILE
1	E	52	LEU

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Mol	Chain	Res	Type
1	E	66	SER
1	E	165	GLN
1	E	180	LYS
2	Q	364	LEU
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	478	LEU
2	Q	507	LYS
1	F	4	LEU
1	F	19	ILE
1	F	52	LEU
1	F	165	GLN
1	F	181	THR
2	R	343	ILE
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	473	LYS
2	R	478	LEU
2	R	497	ASN
2	R	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	59	ASN
1	A	163	GLN
1	A	165	GLN
2	M	359	HIS
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	140	HIS
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	165	GLN
2	N	334	GLN
2	N	359	HIS
2	N	361	HIS
2	N	497	ASN
2	N	503	GLN
1	C	11	GLN
1	C	18	HIS
1	C	87	ASN
1	C	163	GLN
1	C	165	GLN
2	O	361	HIS
2	O	497	ASN
2	O	503	GLN
2	O	530	GLN
1	D	163	GLN
1	D	165	GLN
2	P	305	ASN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	530	GLN
1	E	18	HIS
1	E	163	GLN
1	E	165	GLN
2	Q	305	ASN
2	Q	361	HIS
2	Q	394	ASN
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
2	Q	530	GLN
1	F	11	GLN
1	F	115	ASN
1	F	163	GLN
1	F	165	GLN
2	R	361	HIS
2	R	394	ASN
2	R	422	ASN
2	R	497	ASN
2	R	514	ASN
2	R	530	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DHB	M	551	-	11,11,11	1.19	0	15,15,15	1.44	3 (20%)
5	DHB	R	550	3	11,11,11	1.42	3 (27%)	15,15,15	1.25	2 (13%)
5	DHB	R	551	-	11,11,11	1.22	1 (9%)	15,15,15	1.24	3 (20%)
5	DHB	P	551	-	11,11,11	1.30	1 (9%)	15,15,15	1.34	3 (20%)
5	DHB	N	602	-	11,11,11	1.09	0	15,15,15	1.22	2 (13%)
5	DHB	Q	551	-	11,11,11	1.28	0	15,15,15	1.29	2 (13%)
4	BME	N	601	2	3,3,3	0.19	0	2,2,2	0.25	0
4	BME	M	601	2	3,3,3	0.23	0	2,2,2	0.15	0
5	DHB	M	550	3	11,11,11	1.33	1 (9%)	15,15,15	1.20	2 (13%)
4	BME	R	601	2	3,3,3	0.64	0	2,2,2	0.79	0
4	BME	P	601	2	3,3,3	0.39	0	2,2,2	0.74	0
5	DHB	P	550	3	11,11,11	1.34	1 (9%)	15,15,15	1.31	2 (13%)
4	BME	Q	601	2	3,3,3	0.36	0	2,2,2	0.34	0
5	DHB	Q	550	3	11,11,11	1.45	2 (18%)	15,15,15	1.17	2 (13%)
5	DHB	N	550	3	11,11,11	1.40	3 (27%)	15,15,15	1.36	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DHB	N	551	-	11,11,11	1.20	0	15,15,15	1.17	2 (13%)
4	BME	O	601	2	3,3,3	0.47	0	2,2,2	0.34	0
5	DHB	O	550	3	11,11,11	1.56	3 (27%)	15,15,15	1.32	2 (13%)

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	M	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
5	DHB	P	551	-	-	0/4/4/4	0/1/1/1
5	DHB	N	602	-	-	0/4/4/4	0/1/1/1
5	DHB	Q	551	-	-	0/4/4/4	0/1/1/1
4	BME	N	601	2	-	0/1/1/1	-
4	BME	M	601	2	-	1/1/1/1	-
5	DHB	M	550	3	-	0/4/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	-
4	BME	P	601	2	-	0/1/1/1	-
5	DHB	P	550	3	-	0/4/4/4	0/1/1/1
4	BME	Q	601	2	-	0/1/1/1	-
5	DHB	Q	550	3	-	0/4/4/4	0/1/1/1
5	DHB	N	550	3	-	0/4/4/4	0/1/1/1
5	DHB	N	551	-	-	0/4/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	-
5	DHB	O	550	3	-	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	3.10	1.42	1.36
5	O	550	DHB	C6-C1	2.80	1.43	1.39
5	O	550	DHB	O4-C4	2.69	1.41	1.36
5	Q	550	DHB	C2-C1	2.58	1.43	1.39
5	M	550	DHB	C6-C1	2.41	1.43	1.39
5	N	550	DHB	O4-C4	2.40	1.41	1.36
5	N	550	DHB	C6-C1	2.30	1.42	1.39
5	R	550	DHB	C6-C1	2.27	1.42	1.39
5	N	550	DHB	C2-C3	2.24	1.42	1.38
5	R	550	DHB	C2-C1	2.17	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	550	DHB	O2-C	-2.16	1.24	1.30
5	R	551	DHB	O3-C3	2.15	1.40	1.36
5	Q	550	DHB	O4-C4	2.15	1.40	1.36
5	O	550	DHB	O2-C	-2.14	1.24	1.30
5	P	551	DHB	O3-C3	2.05	1.40	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	DHB	O2-C-O1	-3.63	115.55	123.35
5	R	550	DHB	O2-C-O1	-3.35	116.15	123.35
5	P	550	DHB	O2-C-O1	-3.19	116.49	123.35
5	O	550	DHB	O2-C-C1	3.08	122.75	114.84
5	M	551	DHB	O2-C-O1	-3.07	116.75	123.35
5	M	551	DHB	O2-C-C1	3.02	122.59	114.84
5	O	550	DHB	O2-C-O1	-2.97	116.96	123.35
5	P	551	DHB	O2-C-O1	-2.92	117.06	123.35
5	P	551	DHB	O2-C-C1	2.86	122.18	114.84
5	Q	551	DHB	O2-C-C1	2.72	121.82	114.84
5	N	551	DHB	O2-C-C1	2.70	121.77	114.84
5	M	550	DHB	O2-C-C1	2.70	121.77	114.84
5	Q	551	DHB	O2-C-O1	-2.68	117.58	123.35
5	N	550	DHB	O2-C-C1	2.62	121.56	114.84
5	P	550	DHB	O2-C-C1	2.62	121.56	114.84
5	N	551	DHB	O2-C-O1	-2.49	117.99	123.35
5	N	602	DHB	O2-C-O1	-2.49	118.00	123.35
5	R	550	DHB	O2-C-C1	2.38	120.94	114.84
5	N	602	DHB	O2-C-C1	2.37	120.91	114.84
5	Q	550	DHB	O2-C-O1	-2.29	118.43	123.35
5	M	550	DHB	O2-C-O1	-2.26	118.49	123.35
5	M	551	DHB	C6-C5-C4	-2.25	118.25	120.50
5	Q	550	DHB	O2-C-C1	2.21	120.50	114.84
5	R	551	DHB	O2-C-C1	2.08	120.19	114.84
5	R	551	DHB	C6-C5-C4	-2.07	118.43	120.50
5	R	551	DHB	O2-C-O1	-2.04	118.97	123.35
5	P	551	DHB	C6-C5-C4	-2.02	118.48	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.

4 monomers are involved in 5 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.