



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:10 PM GMT

PDB ID : 3PCI  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 3-iodo-4-HYDROXYBENZOATE  
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.  
Deposited on : 1997-07-02  
Resolution : 2.21 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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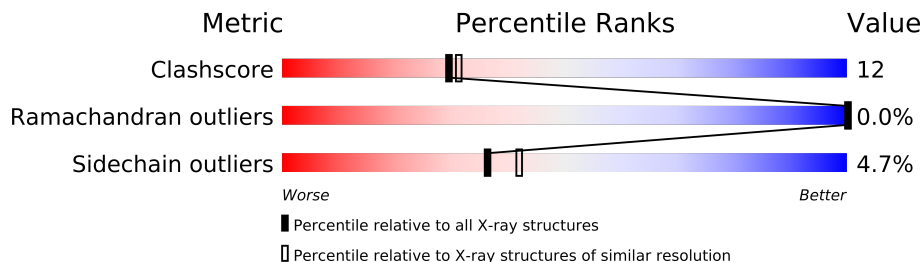
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.21 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	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	
2	M	238	
2	N	238	
2	O	238	
2	P	238	
2	Q	238	
2	R	238	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22104 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

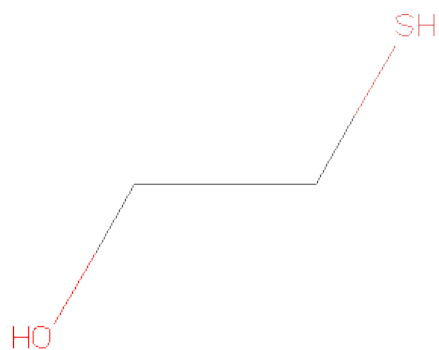
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

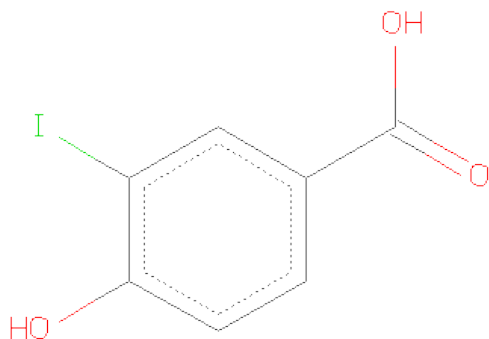
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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-iodo-4-hydroxybenzoic acid (three-letter code: IHB) (formula:  $C_7H_5IO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	I	O	0	0
			11	7	1	3		
5	M	1	Total	C	I	O	0	0
			11	7	1	3		
5	N	1	Total	C	I	O	0	0
			11	7	1	3		
5	N	1	Total	C	I	O	0	0
			11	7	1	3		
5	O	1	Total	C	I	O	0	0
			11	7	1	3		
5	O	1	Total	C	I	O	0	0
			11	7	1	3		
5	P	1	Total	C	I	O	0	0
			11	7	1	3		
5	P	1	Total	C	I	O	0	0
			11	7	1	3		
5	Q	1	Total	C	I	O	0	0
			11	7	1	3		
5	Q	1	Total	C	I	O	0	0
			11	7	1	3		
5	R	1	Total	C	I	O	0	0
			11	7	1	3		
5	R	1	Total	C	I	O	0	0
			11	7	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total 82	O 82	0	0
6	B	85	Total 85	O 85	0	0
6	C	82	Total 82	O 82	0	0
6	D	81	Total 81	O 81	0	0
6	E	84	Total 84	O 84	0	0
6	F	81	Total 81	O 81	0	0
6	M	163	Total 163	O 163	0	0
6	N	167	Total 167	O 167	0	0
6	O	162	Total 162	O 162	0	0
6	P	157	Total 157	O 157	0	0
6	Q	165	Total 165	O 165	0	0
6	R	167	Total 167	O 167	0	0

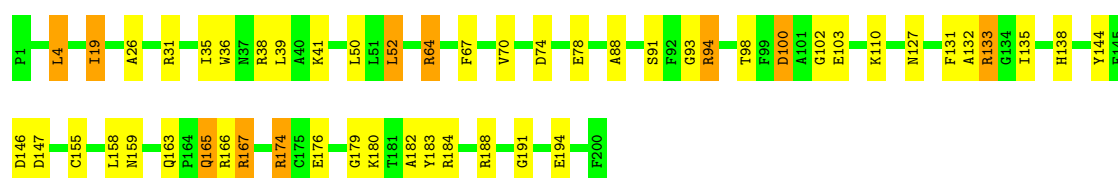
### 3 Residue-property plots

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

Note EDS was not executed.

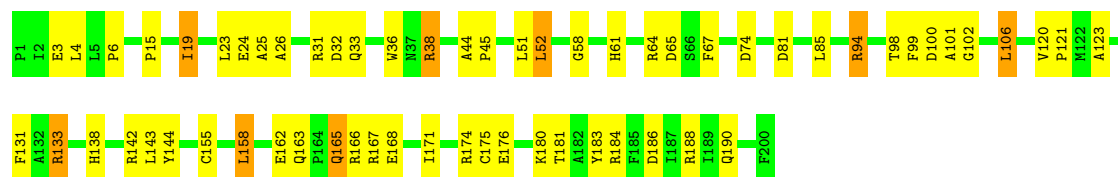
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



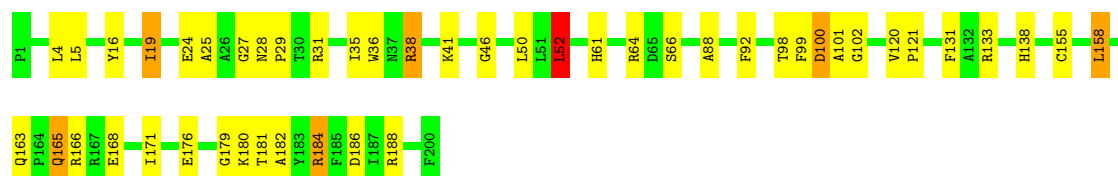
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



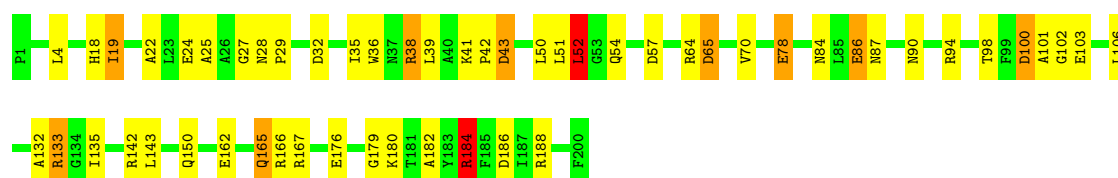
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



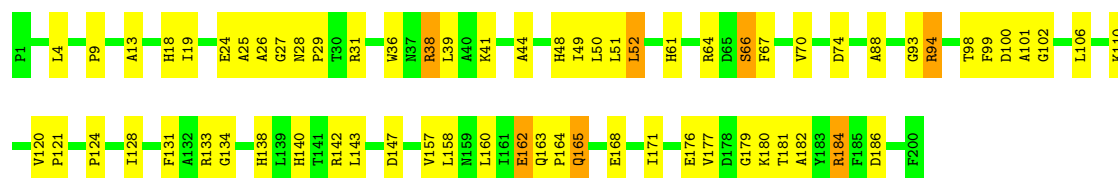
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 



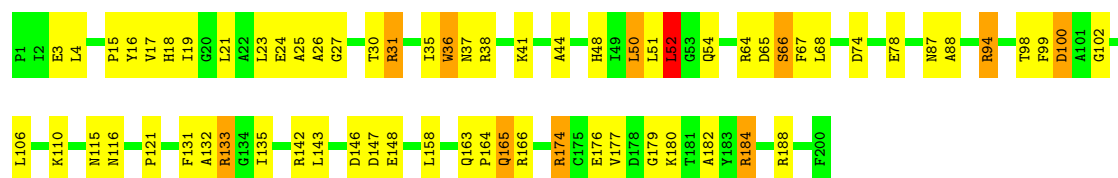
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:



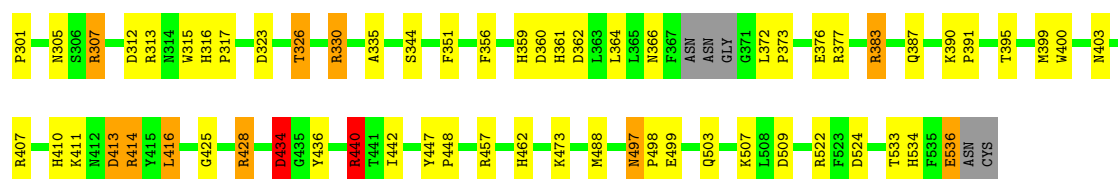
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:



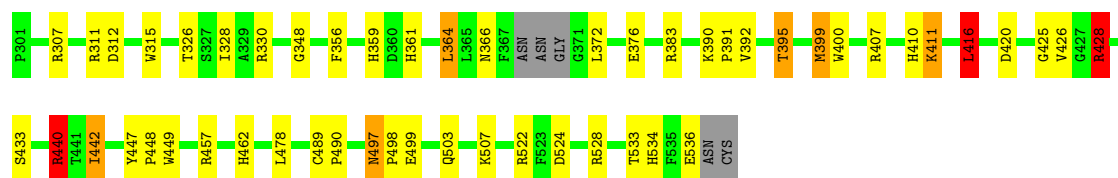
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:



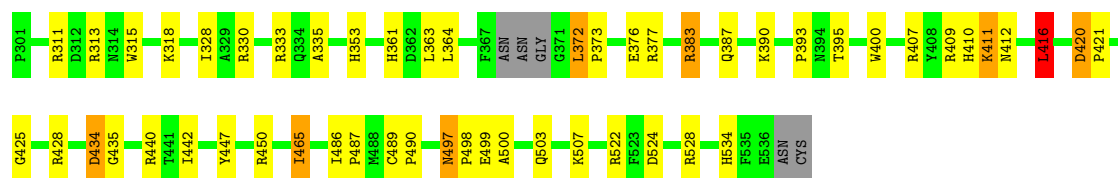
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N:



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:

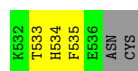


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.00Å 127.07Å 134.08Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	6.00 – 2.21	Depositor
% Data completeness (in resolution range)	83.0 (6.00-2.21)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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: IHB, FE, BME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.94	1/1611 (0.1%)	1.66	30/2195 (1.4%)
1	B	0.95	0/1611	1.66	33/2195 (1.5%)
1	C	0.95	1/1611 (0.1%)	1.50	14/2195 (0.6%)
1	D	0.92	0/1611	1.52	23/2195 (1.0%)
1	E	0.97	0/1611	1.52	23/2195 (1.0%)
1	F	0.98	0/1611	1.55	25/2195 (1.1%)
2	M	1.00	0/1895	1.54	25/2580 (1.0%)
2	N	0.98	0/1895	1.50	16/2580 (0.6%)
2	O	1.00	0/1895	1.55	24/2580 (0.9%)
2	P	0.97	0/1895	1.53	21/2580 (0.8%)
2	Q	1.02	1/1895 (0.1%)	1.54	24/2580 (0.9%)
2	R	1.00	1/1895 (0.1%)	1.56	24/2580 (0.9%)
All	All	0.98	4/21036 (0.0%)	1.55	282/28650 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-5.16	1.37	1.46
1	C	66	SER	CB-OG	-5.10	1.35	1.42
2	R	428	ARG	CD-NE	-5.07	1.37	1.46
2	Q	433	SER	CB-OG	5.05	1.48	1.42

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	440	ARG	NE-CZ-NH2	-20.04	110.28	120.30
2	P	440	ARG	NE-CZ-NH2	-19.34	110.63	120.30
2	R	440	ARG	NE-CZ-NH2	-18.26	111.17	120.30
2	M	440	ARG	NE-CZ-NH2	-16.43	112.08	120.30
2	Q	440	ARG	NE-CZ-NH2	-15.94	112.33	120.30
2	P	440	ARG	NE-CZ-NH1	15.59	128.10	120.30
1	B	184	ARG	NE-CZ-NH2	-15.52	112.54	120.30
1	A	94	ARG	NE-CZ-NH1	14.84	127.72	120.30
1	A	94	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	B	94	ARG	NE-CZ-NH1	13.71	127.16	120.30
1	A	133	ARG	NE-CZ-NH1	13.70	127.15	120.30
2	O	440	ARG	NE-CZ-NH2	-13.09	113.76	120.30
2	Q	457	ARG	NE-CZ-NH1	12.93	126.77	120.30
2	O	428	ARG	CD-NE-CZ	12.68	141.36	123.60
2	N	440	ARG	NE-CZ-NH1	10.82	125.71	120.30
2	M	457	ARG	CD-NE-CZ	10.76	138.67	123.60
2	O	528	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	B	188	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	188	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	C	188	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	B	94	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	B	38	ARG	NE-CZ-NH2	-10.34	115.13	120.30
2	Q	457	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	M	428	ARG	CD-NE-CZ	10.05	137.67	123.60
2	M	428	ARG	NE-CZ-NH2	-9.99	115.31	120.30
2	R	311	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	R	307	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	184	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	O	330	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	B	133	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	C	166	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	133	ARG	NE-CZ-NH2	-9.63	115.49	120.30
2	R	428	ARG	CD-NE-CZ	9.61	137.06	123.60
2	O	524	ASP	CB-CG-OD1	9.51	126.85	118.30
1	F	142	ARG	NE-CZ-NH1	9.49	125.04	120.30
2	Q	522	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	D	184	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	184	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	C	184	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	Q	440	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	B	133	ARG	CD-NE-CZ	9.09	136.32	123.60
1	F	166	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	E	184	ARG	NE-CZ-NH2	-8.98	115.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	457	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	188	ARG	NE-CZ-NH2	-8.95	115.83	120.30
2	P	307	ARG	NE-CZ-NH1	8.91	124.76	120.30
2	R	383	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	O	333	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	188	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	D	94	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	184	ARG	NE-CZ-NH2	-8.86	115.87	120.30
2	O	428	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	D	167	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	F	94	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	F	38	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	F	166	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	D	52	LEU	CB-CA-C	8.68	126.69	110.20
2	R	428	ARG	NE-CZ-NH2	-8.66	115.97	120.30
2	M	428	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	F	38	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	R	307	ARG	NE-CZ-NH2	-8.27	116.16	120.30
2	Q	428	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	C	166	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	E	184	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	O	528	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	D	65	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	133	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	174	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	166	ARG	NE-CZ-NH1	8.03	124.31	120.30
2	M	440	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	E	52	LEU	CB-CA-C	7.96	125.32	110.20
2	O	383	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	R	524	ASP	CB-CG-OD1	7.91	125.42	118.30
1	E	38	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	C	38	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	B	184	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	188	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	R	531	ARG	NE-CZ-NH2	-7.83	116.38	120.30
2	O	409	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	P	509	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	166	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	N	428	ARG	CG-CD-NE	7.71	127.98	111.80
1	E	31	ARG	NE-CZ-NH1	7.70	124.15	120.30
2	M	414	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	Q	383	ARG	NE-CZ-NH2	-7.63	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	353	HIS	CA-CB-CG	-7.62	100.66	113.60
1	A	31	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	74	ASP	CB-CG-OD2	-7.60	111.46	118.30
2	N	528	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	74	ASP	CB-CG-OD1	7.48	125.03	118.30
2	Q	313	ARG	NE-CZ-NH1	7.47	124.04	120.30
2	M	312	ASP	CB-CG-OD1	7.47	125.02	118.30
2	M	383	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	M	407	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	38	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	R	428	ARG	CG-CD-NE	7.39	127.33	111.80
1	C	52	LEU	CB-CA-C	7.38	124.22	110.20
1	B	167	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	31	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	43	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	B	31	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	O	528	ARG	CD-NE-CZ	7.08	133.51	123.60
2	O	377	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	P	432	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	64	ARG	NE-CZ-NH1	-7.01	116.79	120.30
2	P	457	ARG	CD-NE-CZ	6.99	133.39	123.60
2	M	307	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	142	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	Q	528	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	F	38	ARG	CA-CB-CG	6.96	128.70	113.40
2	P	536	GLU	CA-C-O	6.96	134.71	120.10
1	D	133	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	C	133	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	P	414	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	F	142	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	133	ARG	CD-NE-CZ	6.88	133.22	123.60
1	B	133	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	E	74	ASP	CB-CG-OD2	-6.87	112.12	118.30
2	Q	428	ARG	NE-CZ-NH1	6.83	123.71	120.30
2	Q	524	ASP	CB-CG-OD1	6.82	124.44	118.30
2	N	407	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	O	434	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	E	74	ASP	CB-CG-OD1	6.76	124.38	118.30
2	M	312	ASP	CB-CG-OD2	-6.75	112.22	118.30
2	N	312	ASP	CB-CG-OD1	6.72	124.35	118.30
1	B	31	ARG	CD-NE-CZ	6.68	132.95	123.60
1	E	94	ARG	NE-CZ-NH1	6.66	123.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	31	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	F	94	ARG	CD-NE-CZ	6.59	132.83	123.60
2	O	428	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	Q	432	ASP	CB-CG-OD1	6.57	124.21	118.30
2	O	420	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	186	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	162	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	94	ARG	CB-CG-CD	6.50	128.49	111.60
1	E	158	LEU	CB-CA-C	6.50	122.54	110.20
1	A	184	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	P	428	ARG	CG-CD-NE	6.44	125.32	111.80
1	A	52	LEU	CA-CB-CG	6.43	130.10	115.30
1	F	94	ARG	CG-CD-NE	6.42	125.28	111.80
1	E	94	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	D	186	ASP	CB-CG-OD1	6.38	124.04	118.30
2	M	536	GLU	CA-C-O	6.36	133.46	120.10
2	R	517	ASP	CB-CG-OD1	6.36	124.03	118.30
2	M	509	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	188	ARG	NE-CZ-NH2	-6.33	117.13	120.30
2	M	330	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	R	428	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	N	311	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	P	524	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	86	GLU	CG-CD-OE1	6.25	130.80	118.30
2	M	524	ASP	CB-CG-OD1	6.25	123.92	118.30
2	P	509	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	94	ARG	CB-CG-CD	6.24	127.83	111.60
2	R	333	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	N	428	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	N	524	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	142	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	166	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	R	383	ARG	NH1-CZ-NH2	6.19	126.21	119.40
2	O	333	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	P	414	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	O	407	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	F	106	LEU	CA-CB-CG	6.17	129.48	115.30
2	R	432	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	F	174	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	N	383	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	P	524	ASP	CB-CG-OD1	6.12	123.81	118.30
2	M	313	ARG	NE-CZ-NH1	6.11	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	386	ASP	CB-CA-C	6.10	122.59	110.40
1	D	166	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	F	31	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	P	483	ASP	CB-CG-OD2	6.07	123.76	118.30
2	Q	409	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	94	ARG	CG-CD-NE	6.05	124.51	111.80
1	A	52	LEU	CB-CA-C	6.04	121.67	110.20
1	B	94	ARG	CG-CD-NE	6.04	124.47	111.80
1	A	94	ARG	CD-NE-CZ	6.03	132.04	123.60
2	M	428	ARG	CG-CD-NE	6.03	124.45	111.80
2	Q	311	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	186	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	167	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	E	36	TRP	CB-CA-C	5.99	122.38	110.40
2	Q	361	HIS	CA-CB-CG	-5.98	103.44	113.60
2	R	362	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	188	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	Q	434	ASP	CB-CG-OD2	-5.97	112.93	118.30
2	Q	360	ASP	CB-CG-OD2	-5.93	112.96	118.30
2	O	409	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	R	428	ARG	CB-CG-CD	5.91	126.96	111.60
1	F	94	ARG	CB-CG-CD	5.90	126.94	111.60
1	A	64	ARG	CD-NE-CZ	-5.85	115.41	123.60
1	B	166	ARG	CD-NE-CZ	5.83	131.77	123.60
2	R	407	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	E	94	ARG	CG-CD-NE	5.83	124.03	111.80
1	F	31	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	R	440	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	142	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	186	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	Q	377	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	166	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	N	383	ARG	CD-NE-CZ	-5.75	115.55	123.60
2	O	311	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	52	LEU	CB-CA-C	5.73	121.09	110.20
1	F	184	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	N	457	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	133	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	31	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	36	TRP	CB-CA-C	5.68	121.75	110.40
1	B	186	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	M	313	ARG	CB-CA-C	5.62	121.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	440	ARG	NH1-CZ-NH2	5.62	125.58	119.40
2	Q	457	ARG	CA-CB-CG	5.61	125.73	113.40
1	B	52	LEU	CA-CB-CG	5.60	128.17	115.30
2	M	413	ASP	CB-CG-OD1	5.59	123.33	118.30
2	M	434	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	R	361	HIS	CA-CB-CG	-5.57	104.12	113.60
2	N	457	ARG	CA-CB-CG	5.57	125.66	113.40
1	B	133	ARG	CA-CB-CG	5.57	125.66	113.40
1	C	66	SER	N-CA-CB	5.56	118.84	110.50
1	D	38	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	P	361	HIS	CA-CB-CG	-5.52	104.22	113.60
1	F	74	ASP	CB-CG-OD1	5.49	123.24	118.30
2	P	519	LEU	CB-CA-C	5.48	120.61	110.20
1	F	52	LEU	CB-CA-C	5.48	120.61	110.20
1	F	66	SER	N-CA-CB	5.46	118.70	110.50
1	E	31	ARG	CD-NE-CZ	5.46	131.24	123.60
2	Q	360	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	133	ARG	CA-CB-CG	5.44	125.36	113.40
1	B	32	ASP	CB-CG-OD1	5.44	123.19	118.30
2	O	416	LEU	CB-CA-C	5.43	120.51	110.20
1	A	36	TRP	CB-CA-C	5.42	121.24	110.40
2	N	416	LEU	CB-CA-C	5.41	120.49	110.20
1	E	66	SER	N-CA-CB	5.41	118.62	110.50
1	A	103	GLU	CG-CD-OE1	-5.37	107.55	118.30
1	F	38	ARG	CB-CA-C	5.36	121.12	110.40
1	B	175	CYS	CA-CB-SG	5.36	123.64	114.00
1	F	36	TRP	CB-CA-C	5.36	121.11	110.40
1	F	158	LEU	CB-CA-C	5.35	120.37	110.20
2	R	434	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	E	140	HIS	CB-CA-C	-5.34	99.71	110.40
1	D	57	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	36	TRP	CB-CA-C	5.33	121.06	110.40
1	D	100	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	B	74	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	Q	407	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	O	440	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	F	146	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	133	ARG	CA-CB-CG	5.29	125.03	113.40
1	D	32	ASP	CB-CG-OD1	5.28	123.06	118.30
1	E	38	ARG	CD-NE-CZ	-5.28	116.22	123.60
1	D	32	ASP	CB-CG-OD2	-5.27	113.56	118.30
2	Q	452	GLY	N-CA-C	-5.26	99.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	GLU	CG-CD-OE1	-5.26	107.79	118.30
2	R	352	SER	N-CA-CB	5.24	118.36	110.50
2	O	500	ALA	CB-CA-C	5.23	117.95	110.10
1	A	146	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	P	307	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	R	330	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	36	TRP	CB-CA-C	5.21	120.83	110.40
1	A	183	TYR	N-CA-CB	5.18	119.93	110.60
2	P	376	GLU	CG-CD-OE1	5.17	128.64	118.30
2	M	323	ASP	CB-CG-OD1	5.16	122.94	118.30
2	M	524	ASP	CB-CG-OD2	-5.15	113.67	118.30
2	O	313	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	100	ASP	CB-CG-OD2	5.14	122.93	118.30
2	P	455	ASP	CB-CG-OD1	5.13	122.91	118.30
2	N	383	ARG	N-CA-CB	-5.12	101.39	110.60
2	Q	372	LEU	N-CA-CB	-5.11	100.19	110.40
1	B	24	GLU	CA-CB-CG	5.09	124.60	113.40
1	F	23	LEU	CB-CA-C	5.08	119.85	110.20
2	Q	383	ARG	N-CA-CB	-5.07	101.48	110.60
1	E	133	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	M	326	THR	CA-CB-OG1	-5.06	98.36	109.00
2	N	420	ASP	CB-CG-OD1	5.06	122.85	118.30
1	E	13	ALA	CB-CA-C	5.04	117.66	110.10
1	D	78	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	B	162	GLU	CG-CD-OE1	-5.02	108.26	118.30
1	B	183	TYR	N-CA-CB	5.02	119.63	110.60
1	B	174	ARG	CD-NE-CZ	-5.01	116.58	123.60
2	P	478	LEU	CA-CB-CG	5.01	126.82	115.30
1	E	186	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	184	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	37	0
1	B	1571	0	1499	40	0
1	C	1571	0	1499	29	1
1	D	1571	0	1499	35	2
1	E	1571	0	1499	47	0
1	F	1571	0	1499	66	0
2	M	1840	0	1792	57	0
2	N	1840	0	1792	39	0
2	O	1840	0	1792	36	0
2	P	1840	0	1792	41	0
2	Q	1840	0	1792	56	0
2	R	1840	0	1792	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	1	0
4	N	4	0	5	0	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	2	0
4	R	4	0	5	0	0
5	M	22	0	7	1	0
5	N	22	0	7	1	0
5	O	22	0	7	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	3	0
6	A	82	0	0	0	0
6	B	85	0	0	0	0
6	C	82	0	0	0	1
6	D	81	0	0	0	0
6	E	84	0	0	2	0
6	F	81	0	0	2	0
6	M	163	0	0	7	0
6	N	167	0	0	3	0
6	O	162	0	0	6	0
6	P	157	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	165	0	0	8	1
6	R	167	0	0	4	0
All	All	22104	0	19818	492	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (492) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.25	1.16
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.22	1.12
1:D:64:ARG:NH1	1:D:100:ASP:O	1.81	1.12
1:B:165:GLN:NE2	1:B:165:GLN:H	1.49	1.10
1:F:165:GLN:NE2	1:F:165:GLN:H	1.50	1.09
1:F:64:ARG:NH1	1:F:100:ASP:O	1.88	1.07
1:E:165:GLN:NE2	1:E:165:GLN:H	1.54	1.04
1:A:165:GLN:H	1:A:165:GLN:NE2	1.56	1.02
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.59	1.00
1:C:165:GLN:H	1:C:165:GLN:NE2	1.60	0.99
1:C:64:ARG:NH1	1:C:100:ASP:O	1.94	0.99
1:E:165:GLN:N	1:E:165:GLN:HE21	1.61	0.98
1:C:99:PHE:HE2	2:O:411:LYS:HZ3	1.11	0.92
2:R:361:HIS:H	2:R:361:HIS:CD2	1.87	0.92
1:B:165:GLN:HE21	1:B:165:GLN:H	1.05	0.92
1:D:165:GLN:H	1:D:165:GLN:HE21	1.05	0.92
1:F:165:GLN:HE21	1:F:165:GLN:H	1.16	0.91
2:M:497:ASN:ND2	2:M:499:GLU:H	1.69	0.90
1:A:165:GLN:H	1:A:165:GLN:HE21	1.11	0.90
1:C:165:GLN:H	1:C:165:GLN:HE21	1.12	0.90
1:C:25:ALA:O	2:O:411:LYS:NZ	2.03	0.89
2:P:364:LEU:CD2	2:P:440:ARG:HD3	2.00	0.89
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.38	0.89
2:M:522:ARG:NH1	6:M:665:HOH:O	2.07	0.88
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.71	0.88
1:D:165:GLN:H	1:D:165:GLN:NE2	1.73	0.86
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.05	0.86
2:R:497:ASN:ND2	2:R:499:GLU:H	1.73	0.86
2:N:390:LYS:HD2	6:N:649:HOH:O	1.75	0.86
1:A:64:ARG:NH1	1:A:100:ASP:O	2.09	0.85
1:B:25:ALA:O	2:N:411:LYS:NZ	2.10	0.84
1:D:176:GLU:OE2	1:D:179:GLY:HA2	1.76	0.84
2:M:390:LYS:HD2	6:M:642:HOH:O	1.78	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:361:HIS:H	2:Q:361:HIS:CD2	1.95	0.83
2:O:390:LYS:HD2	6:O:653:HOH:O	1.79	0.82
2:N:364:LEU:HD22	2:N:440:ARG:HD3	1.61	0.82
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.60	0.82
1:F:165:GLN:HE21	1:F:165:GLN:N	1.76	0.81
2:P:390:LYS:HD3	6:P:650:HOH:O	1.80	0.81
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.28	0.80
1:F:25:ALA:O	2:R:411:LYS:NZ	2.13	0.80
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.46	0.80
2:M:497:ASN:HD22	2:M:499:GLU:H	1.26	0.80
1:B:165:GLN:N	1:B:165:GLN:HE21	1.79	0.80
1:B:176:GLU:HG3	1:B:180:LYS:O	1.82	0.80
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.48	0.79
1:F:176:GLU:HG3	1:F:180:LYS:O	1.82	0.79
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.83	0.78
2:R:497:ASN:HD22	2:R:499:GLU:H	1.30	0.78
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.67	0.77
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.67	0.77
5:Q:550:IHB:H2	6:Q:1225:HOH:O	1.84	0.77
2:O:497:ASN:ND2	2:O:499:GLU:H	1.82	0.76
2:R:361:HIS:H	2:R:361:HIS:HD2	1.32	0.76
2:P:497:ASN:HD22	2:P:497:ASN:C	1.89	0.76
2:M:305:ASN:O	2:M:533:THR:HG23	1.84	0.76
1:C:165:GLN:N	1:C:165:GLN:HE21	1.83	0.76
2:P:361:HIS:CD2	2:P:361:HIS:H	2.04	0.75
2:P:497:ASN:ND2	2:P:499:GLU:H	1.85	0.75
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.68	0.73
1:A:165:GLN:N	1:A:165:GLN:HE21	1.85	0.73
2:M:315:TRP:HZ2	2:M:503:GLN:HE21	1.35	0.73
1:C:98:THR:OG1	1:C:102:GLY:N	2.21	0.73
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.89	0.73
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.23	0.73
1:F:50:LEU:HD12	1:F:51:LEU:N	2.03	0.72
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.25	0.72
1:A:98:THR:OG1	1:A:102:GLY:N	2.22	0.72
2:N:522:ARG:NH1	6:N:671:HOH:O	2.22	0.72
1:E:64:ARG:NH1	1:E:100:ASP:O	2.22	0.71
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.22	0.70
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.15	0.70
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.73	0.69
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.40	0.69
1:F:165:GLN:NE2	1:F:165:GLN:N	2.31	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:THR:HB	1:A:100:ASP:OD1	1.93	0.69
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.56	0.69
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.75	0.69
2:R:304:ASP:HB2	2:R:343:ILE:HB	1.75	0.69
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.75	0.68
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	1.91	0.68
1:F:163:GLN:HB3	1:F:165:GLN:NE2	2.07	0.68
1:D:165:GLN:N	1:D:165:GLN:HE21	1.87	0.68
1:B:65:ASP:OD2	1:B:133:ARG:HD3	1.94	0.68
1:E:165:GLN:H	1:E:165:GLN:HE21	0.76	0.68
2:M:361:HIS:H	2:M:361:HIS:CD2	2.11	0.68
2:Q:497:ASN:HD22	2:Q:497:ASN:C	1.97	0.67
2:N:361:HIS:H	2:N:361:HIS:CD2	2.13	0.67
1:F:26:ALA:C	2:R:411:LYS:HZ2	1.98	0.67
1:F:188:ARG:HG3	1:F:188:ARG:HH11	1.60	0.67
1:E:134:GLY:HA3	2:Q:326:THR:HG22	1.77	0.66
1:E:98:THR:OG1	1:E:102:GLY:N	2.29	0.66
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.78	0.66
1:D:84:ASN:OD1	1:D:86:GLU:HB2	1.96	0.66
1:E:99:PHE:HE2	2:Q:411:LYS:NZ	1.93	0.66
2:P:390:LYS:HE2	6:P:726:HOH:O	1.95	0.65
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.31	0.65
1:F:98:THR:OG1	1:F:102:GLY:N	2.27	0.65
2:N:416:LEU:C	2:N:416:LEU:HD23	2.17	0.65
2:N:315:TRP:HZ2	2:N:503:GLN:HE21	1.45	0.65
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.78	0.64
1:D:100:ASP:N	1:D:100:ASP:OD1	2.27	0.64
2:O:361:HIS:CD2	2:O:361:HIS:H	2.14	0.64
2:Q:536:GLU:HB2	6:Q:1142:HOH:O	1.97	0.64
1:B:99:PHE:HE2	2:N:411:LYS:NZ	1.96	0.64
2:M:360:ASP:OD2	2:M:428:ARG:HD2	1.98	0.64
2:R:522:ARG:NH1	6:R:1345:HOH:O	2.24	0.64
2:R:400:TRP:HA	2:R:425:GLY:O	1.98	0.63
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.32	0.63
2:Q:497:ASN:HD22	2:Q:498:PRO:N	1.96	0.63
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.96	0.63
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.29	0.63
1:B:165:GLN:N	1:B:165:GLN:NE2	2.34	0.63
1:F:99:PHE:HE2	2:R:411:LYS:HZ3	1.46	0.63
2:Q:376:GLU:OE1	6:Q:1049:HOH:O	2.15	0.62
2:O:416:LEU:C	2:O:416:LEU:HD23	2.19	0.62
1:F:100:ASP:N	1:F:100:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:497:ASN:HD22	2:O:498:PRO:N	1.97	0.62
2:O:497:ASN:HD22	2:O:499:GLU:H	1.47	0.61
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.80	0.61
2:M:315:TRP:CZ2	2:M:503:GLN:NE2	2.68	0.61
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.83	0.61
1:B:176:GLU:HG3	1:B:180:LYS:C	2.20	0.61
2:Q:450:ARG:NE	6:Q:1470:HOH:O	2.18	0.61
2:Q:383:ARG:HG3	2:Q:436:TYR:CE1	2.36	0.61
1:F:110:LYS:NZ	1:F:148:GLU:OE2	2.25	0.61
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.81	0.60
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.83	0.60
2:O:497:ASN:HD22	2:O:497:ASN:C	2.05	0.60
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.82	0.60
1:F:188:ARG:HG3	1:F:188:ARG:NH1	2.17	0.60
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.44	0.60
2:M:400:TRP:HA	2:M:425:GLY:O	2.02	0.60
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.37	0.60
2:P:497:ASN:HD22	2:P:499:GLU:H	1.48	0.59
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.17	0.59
2:P:361:HIS:HD2	2:P:361:HIS:H	1.50	0.59
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.01	0.59
2:R:447:TYR:OH	5:R:550:IHB:O4	2.20	0.59
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.85	0.59
5:M:550:IHB:H2	6:M:742:HOH:O	2.03	0.59
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.03	0.59
1:D:176:GLU:HG3	1:D:180:LYS:O	2.02	0.59
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.68	0.59
1:B:98:THR:OG1	1:B:102:GLY:N	2.35	0.59
1:A:176:GLU:HA	1:A:180:LYS:O	2.03	0.58
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.36	0.58
1:C:100:ASP:OD1	1:C:100:ASP:N	2.36	0.58
1:A:165:GLN:N	1:A:165:GLN:NE2	2.41	0.58
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.83	0.58
2:P:497:ASN:HD22	2:P:498:PRO:N	2.00	0.58
2:O:376:GLU:O	2:O:442:ILE:HA	2.03	0.58
2:R:413:ASP:C	2:R:414:ARG:HD2	2.24	0.58
1:D:25:ALA:O	2:P:411:LYS:NZ	2.37	0.58
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.04	0.58
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.04	0.58
1:E:98:THR:O	1:E:102:GLY:HA2	2.04	0.57
1:F:41:LYS:HE3	1:F:87:ASN:O	2.04	0.57
1:E:99:PHE:CE2	2:Q:411:LYS:NZ	2.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:24:GLU:O	1:F:27:GLY:N	2.35	0.57
1:E:143:LEU:HD23	1:E:143:LEU:C	2.25	0.57
1:E:25:ALA:O	2:Q:411:LYS:NZ	2.37	0.57
1:E:176:GLU:HG3	1:E:180:LYS:O	2.04	0.57
2:N:364:LEU:HD22	2:N:440:ARG:CD	2.34	0.57
2:P:416:LEU:HD23	2:P:416:LEU:C	2.25	0.57
1:F:50:LEU:O	1:F:182:ALA:HA	2.05	0.57
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.69	0.57
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.87	0.57
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.49	0.56
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.40	0.56
1:B:15:PRO:HB3	1:B:133:ARG:HD2	1.85	0.56
1:F:54:GLN:HG2	1:F:102:GLY:O	2.06	0.56
1:B:64:ARG:NH1	1:B:100:ASP:O	2.39	0.56
1:F:143:LEU:HD23	1:F:143:LEU:C	2.24	0.56
2:R:350:ASN:OD1	2:R:352:SER:HB2	2.04	0.56
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.41	0.56
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.37	0.56
1:E:176:GLU:OE2	1:E:179:GLY:CA	2.45	0.56
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.87	0.56
2:R:390:LYS:HD3	6:R:1425:HOH:O	2.05	0.56
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.21	0.55
1:F:165:GLN:CD	1:F:165:GLN:H	1.98	0.55
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.88	0.55
1:D:28:ASN:HB3	1:D:29:PRO:HD2	1.88	0.55
2:N:359:HIS:O	2:N:366:ASN:HB3	2.06	0.55
1:F:98:THR:O	1:F:102:GLY:HA2	2.07	0.55
1:B:19:ILE:O	2:N:426:VAL:HG21	2.06	0.55
2:Q:465:ILE:N	2:Q:465:ILE:HD12	2.22	0.55
2:R:407:ARG:NH1	2:R:417:ALA:O	2.33	0.55
2:R:497:ASN:HD22	2:R:498:PRO:N	2.05	0.55
1:A:26:ALA:C	2:M:411:LYS:HZ2	2.10	0.55
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.42	0.55
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.42	0.55
1:A:50:LEU:O	1:A:182:ALA:HA	2.06	0.54
2:R:315:TRP:HZ2	2:R:503:GLN:NE2	2.03	0.54
2:P:416:LEU:CD2	2:P:416:LEU:C	2.75	0.54
2:M:497:ASN:HD22	2:M:498:PRO:N	2.05	0.54
1:D:50:LEU:O	1:D:182:ALA:HA	2.08	0.54
2:M:361:HIS:HD2	2:M:361:HIS:H	1.55	0.54
1:C:176:GLU:HG3	1:C:180:LYS:O	2.06	0.54
1:F:121:PRO:O	6:F:1400:HOH:O	2.18	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:168:GLU:HA	1:E:171:ILE:CD1	2.37	0.54
2:M:376:GLU:OE1	6:M:637:HOH:O	2.18	0.54
2:O:315:TRP:HE1	2:O:503:GLN:HE22	1.56	0.54
2:N:497:ASN:ND2	2:N:499:GLU:H	2.06	0.54
1:B:168:GLU:HA	1:B:171:ILE:HD12	1.90	0.54
1:C:16:TYR:O	1:C:19:ILE:HG23	2.09	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.09	0.53
1:A:176:GLU:HG3	1:A:180:LYS:O	2.09	0.53
1:D:78:GLU:HG2	2:P:301:PRO:HG2	1.91	0.53
2:O:522:ARG:NH1	6:O:676:HOH:O	2.42	0.53
2:M:536:GLU:HB2	6:M:697:HOH:O	2.08	0.53
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.91	0.52
2:M:434:ASP:HB3	2:M:436:TYR:CD2	2.44	0.52
1:B:180:LYS:HG2	1:B:181:THR:N	2.23	0.52
2:P:400:TRP:HA	2:P:425:GLY:O	2.10	0.52
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.44	0.52
2:R:361:HIS:N	2:R:361:HIS:CD2	2.62	0.52
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.91	0.52
2:M:434:ASP:HB3	2:M:436:TYR:CE2	2.45	0.52
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.45	0.52
1:F:78:GLU:OE2	2:R:301:PRO:HG3	2.09	0.52
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.40	0.52
2:N:376:GLU:O	2:N:442:ILE:HA	2.09	0.52
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.06	0.51
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.30	0.51
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.92	0.51
1:C:24:GLU:O	1:C:27:GLY:N	2.40	0.51
2:M:377:ARG:NH1	2:P:416:LEU:HD21	2.26	0.51
2:N:478:LEU:C	2:N:478:LEU:HD23	2.31	0.51
2:N:416:LEU:C	2:N:416:LEU:CD2	2.78	0.51
2:R:447:TYR:OH	5:R:550:IHB:C4	2.58	0.51
2:R:497:ASN:HD22	2:R:497:ASN:C	2.14	0.51
1:F:50:LEU:C	1:F:50:LEU:HD12	2.30	0.51
2:M:359:HIS:O	2:M:366:ASN:HB3	2.11	0.51
1:E:184:ARG:HG3	1:E:184:ARG:NH1	2.25	0.51
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.31	0.51
1:B:51:LEU:HD12	1:B:106:LEU:HD22	1.93	0.50
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.27	0.50
2:Q:390:LYS:HE2	6:Q:1179:HOH:O	2.11	0.50
2:M:497:ASN:ND2	2:M:499:GLU:N	2.50	0.50
2:Q:522:ARG:NH1	6:Q:1099:HOH:O	2.43	0.50
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:326:THR:HG22	2:P:330:ARG:HD2	1.93	0.50
1:B:6:PRO:HB2	2:N:503:GLN:HE22	1.76	0.50
2:Q:447:TYR:CE1	5:Q:550:IHB:C5	2.95	0.50
2:R:364:LEU:HD11	2:R:442:ILE:HG23	1.93	0.50
1:F:131:PHE:O	1:F:132:ALA:HB2	2.11	0.50
2:N:400:TRP:HA	2:N:425:GLY:O	2.12	0.50
1:D:98:THR:OG1	1:D:102:GLY:N	2.39	0.50
1:B:165:GLN:CD	1:B:165:GLN:H	2.14	0.50
2:M:416:LEU:C	2:M:416:LEU:HD23	2.32	0.50
1:B:99:PHE:HE2	2:N:411:LYS:HZ3	1.58	0.49
2:N:364:LEU:CD2	2:N:440:ARG:HD3	2.36	0.49
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.94	0.49
2:M:497:ASN:HD22	2:M:497:ASN:C	2.16	0.49
2:N:410:HIS:CE1	2:N:411:LYS:HG3	2.47	0.49
1:F:44:ALA:O	1:F:48:HIS:NE2	2.30	0.49
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.47	0.49
5:O:550:IHB:H2	6:O:760:HOH:O	2.11	0.49
2:R:410:HIS:CE1	2:R:411:LYS:HG3	2.47	0.49
1:A:26:ALA:C	2:M:411:LYS:NZ	2.65	0.49
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.13	0.49
1:B:98:THR:O	1:B:102:GLY:HA2	2.13	0.49
2:R:371:GLY:N	2:R:422:ASN:ND2	2.61	0.49
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.30	0.49
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.94	0.49
1:D:24:GLU:O	1:D:27:GLY:N	2.45	0.49
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.76	0.49
1:A:133:ARG:HG2	2:M:326:THR:HG21	1.95	0.49
2:N:497:ASN:HD22	2:N:499:GLU:H	1.61	0.49
2:O:400:TRP:HA	2:O:425:GLY:O	2.13	0.49
2:Q:450:ARG:NH2	6:Q:1470:HOH:O	2.42	0.48
2:R:385:VAL:O	2:R:526:VAL:HA	2.14	0.48
1:F:115:ASN:HA	1:F:121:PRO:HA	1.95	0.48
1:E:70:VAL:HG12	1:E:128:ILE:HG12	1.96	0.48
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.78	0.48
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.48	0.48
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.96	0.48
2:P:497:ASN:C	2:P:497:ASN:ND2	2.63	0.48
1:F:52:LEU:O	1:F:184:ARG:HA	2.14	0.48
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.72	0.48
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.49	0.48
1:B:33:GLN:HG2	1:B:85:LEU:HD12	1.96	0.48
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.72	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.35	0.47
1:B:51:LEU:HD12	1:B:106:LEU:CD2	2.44	0.47
2:N:536:GLU:HB2	6:N:704:HOH:O	2.14	0.47
2:N:447:TYR:OH	5:N:550:IHB:C5	2.62	0.47
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.96	0.47
1:D:100:ASP:CG	1:D:101:ALA:H	2.17	0.47
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.71	0.47
2:O:364:LEU:HD11	2:O:442:ILE:HG23	1.97	0.47
2:O:465:ILE:N	2:O:465:ILE:HD12	2.30	0.47
1:C:98:THR:HG1	1:C:101:ALA:HB3	1.80	0.47
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.72	0.47
2:M:383:ARG:HG3	2:M:436:TYR:CE1	2.49	0.47
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.50	0.47
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.96	0.47
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.79	0.47
2:Q:416:LEU:HD23	2:Q:417:ALA:N	2.30	0.47
1:D:143:LEU:HD23	1:D:143:LEU:C	2.35	0.47
1:F:26:ALA:C	2:R:411:LYS:NZ	2.68	0.47
1:F:52:LEU:CD2	1:F:184:ARG:NH1	2.77	0.47
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.30	0.47
2:O:447:TYR:OH	5:O:550:IHB:C5	2.63	0.47
1:E:165:GLN:NE2	1:E:165:GLN:N	2.38	0.46
2:M:403:ASN:HB2	6:M:610:HOH:O	2.15	0.46
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.63	0.46
2:Q:325:LYS:HG2	2:R:335:ALA:HB1	1.96	0.46
2:R:448:PRO:HD3	2:R:456:TRP:CZ3	2.50	0.46
1:D:98:THR:O	1:D:102:GLY:HA2	2.14	0.46
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	1.97	0.46
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.50	0.46
2:Q:360:ASP:OD2	2:Q:428:ARG:HD2	2.15	0.46
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.15	0.46
2:Q:432:ASP:OD1	2:Q:434:ASP:N	2.38	0.46
1:D:176:GLU:OE2	1:D:179:GLY:CA	2.56	0.46
2:R:414:ARG:N	2:R:414:ARG:HD2	2.30	0.46
1:C:50:LEU:O	1:C:182:ALA:HA	2.16	0.46
1:E:176:GLU:HA	1:E:180:LYS:O	2.16	0.46
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.86	0.46
2:R:356:PHE:CD1	2:R:428:ARG:HD3	2.50	0.46
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.97	0.46
2:M:316:HIS:HB3	2:M:317:PRO:HD2	1.97	0.46
1:F:52:LEU:HD21	1:F:184:ARG:NH1	2.30	0.46
1:B:155:CYS:HB3	1:B:158:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:24:GLU:O	1:D:27:GLY:HA2	2.16	0.46
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.30	0.46
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.98	0.46
1:D:39:LEU:HB3	1:D:90:ASN:O	2.15	0.46
2:R:315:TRP:CZ2	2:R:503:GLN:NE2	2.82	0.45
1:C:98:THR:O	1:C:102:GLY:HA2	2.16	0.45
2:Q:522:ARG:NE	2:Q:524:ASP:OD1	2.49	0.45
1:F:94:ARG:HH22	2:R:398:GLU:CD	2.20	0.45
1:F:68:LEU:HD12	1:F:68:LEU:N	2.31	0.45
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.78	0.45
2:Q:399:MET:HA	2:Q:462:HIS:O	2.17	0.45
2:M:448:PRO:CB	2:P:516:MET:HA	2.46	0.45
2:O:486:ILE:HB	2:O:487:PRO:HD3	1.99	0.45
2:N:356:PHE:CD1	2:N:428:ARG:HD3	2.51	0.45
2:P:308:PHE:HA	2:P:529:GLY:O	2.16	0.45
2:O:410:HIS:ND1	2:O:412:ASN:N	2.52	0.45
2:O:383:ARG:HA	2:O:435:GLY:O	2.17	0.45
1:F:16:TYR:O	1:F:19:ILE:HG12	2.17	0.45
1:E:100:ASP:N	1:E:100:ASP:OD1	2.49	0.45
2:M:361:HIS:CG	4:M:601:BME:H21	2.52	0.45
2:N:361:HIS:HD2	2:N:361:HIS:H	1.62	0.45
2:Q:450:ARG:CZ	6:Q:1470:HOH:O	2.63	0.45
2:Q:522:ARG:HD3	2:Q:522:ARG:HH11	1.52	0.45
1:D:54:GLN:HG3	1:D:184:ARG:HH22	1.82	0.45
2:O:410:HIS:CE1	2:O:412:ASN:HB2	2.52	0.44
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.99	0.44
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.32	0.44
1:F:65:ASP:OD2	1:F:133:ARG:HD3	2.18	0.44
1:C:155:CYS:HB3	1:C:158:LEU:HB2	1.98	0.44
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.16	0.44
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.98	0.44
2:M:376:GLU:O	2:M:442:ILE:HA	2.16	0.44
2:R:383:ARG:NH2	2:R:391:PRO:HG3	2.32	0.44
1:C:98:THR:OG1	1:C:101:ALA:HB3	2.17	0.44
1:E:50:LEU:O	1:E:182:ALA:HA	2.18	0.44
5:R:550:IHB:H2	6:R:1471:HOH:O	2.16	0.44
2:R:359:HIS:O	2:R:366:ASN:HB3	2.17	0.44
1:F:19:ILE:HD11	2:R:408:TYR:HD1	1.83	0.44
2:P:360:ASP:HB3	2:P:428:ARG:HG3	2.00	0.44
1:A:147:ASP:OD2	1:A:174:ARG:HD2	2.18	0.44
2:M:372:LEU:HA	2:M:373:PRO:HD3	1.89	0.44
2:R:486:ILE:HB	2:R:487:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:36:TRP:CG	1:F:37:ASN:N	2.86	0.44
1:E:177:VAL:O	1:E:180:LYS:HB3	2.18	0.44
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.72	0.44
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.79	0.43
2:O:372:LEU:HA	2:O:373:PRO:HD3	1.88	0.43
2:R:390:LYS:HD2	6:R:1307:HOH:O	2.17	0.43
1:D:41:LYS:HD2	1:D:87:ASN:O	2.18	0.43
2:O:318:LYS:HA	2:O:318:LYS:HD3	1.88	0.43
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.48	0.43
2:Q:315:TRP:CZ2	2:Q:503:GLN:NE2	2.85	0.43
1:B:58:GLY:CA	1:B:190:GLN:HB3	2.48	0.43
2:O:410:HIS:CE1	2:O:412:ASN:H	2.31	0.43
1:D:176:GLU:HA	1:D:180:LYS:O	2.18	0.43
1:D:132:ALA:HB3	1:D:135:ILE:HD12	2.00	0.43
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.54	0.43
2:Q:522:ARG:HE	2:Q:524:ASP:CG	2.20	0.43
2:M:448:PRO:HB2	2:P:516:MET:HA	2.00	0.43
1:A:191:GLY:O	1:A:194:GLU:HB2	2.19	0.43
1:A:167:ARG:HD2	1:A:167:ARG:HH11	1.56	0.43
1:B:81:ASP:HB2	2:N:348:GLY:O	2.19	0.43
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.83	0.43
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.34	0.43
1:A:98:THR:O	1:A:102:GLY:HA2	2.19	0.43
2:Q:497:ASN:ND2	2:Q:497:ASN:C	2.70	0.43
1:D:133:ARG:NH2	1:E:162:GLU:OE2	2.52	0.43
1:E:120:VAL:HA	1:E:121:PRO:HD3	1.86	0.43
2:M:413:ASP:C	2:M:414:ARG:HD2	2.39	0.43
2:Q:373:PRO:HB3	2:Q:423:PHE:HB2	1.99	0.43
2:P:497:ASN:ND2	2:P:499:GLU:N	2.61	0.43
1:D:162:GLU:OE2	1:F:133:ARG:NH2	2.51	0.43
2:R:378:ILE:HA	2:R:519:LEU:O	2.19	0.43
1:A:155:CYS:O	1:A:159:ASN:ND2	2.32	0.43
2:O:361:HIS:CG	4:O:601:BME:H21	2.53	0.43
2:P:383:ARG:NE	2:P:434:ASP:O	2.38	0.43
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.70	0.43
2:O:315:TRP:HZ2	2:O:503:GLN:NE2	2.16	0.42
2:N:497:ASN:HD22	2:N:498:PRO:N	2.17	0.42
1:E:163:GLN:HA	1:E:164:PRO:HD3	1.91	0.42
1:B:23:LEU:N	1:B:23:LEU:HD12	2.34	0.42
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.53	0.42
1:B:3:GLU:OE1	1:B:3:GLU:CA	2.67	0.42
1:E:124:PRO:HA	6:E:220:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:44:ALA:O	1:E:48:HIS:NE2	2.37	0.42
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.19	0.42
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.54	0.42
1:A:78:GLU:CD	2:M:301:PRO:HG3	2.39	0.42
1:F:176:GLU:HA	1:F:180:LYS:O	2.19	0.42
2:N:328:ILE:HD12	2:O:335:ALA:HB2	2.01	0.42
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.82	0.42
1:E:168:GLU:CA	1:E:171:ILE:HD12	2.44	0.42
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.71	0.42
1:F:15:PRO:HB3	1:F:133:ARG:HD2	2.00	0.42
2:N:399:MET:HA	2:N:462:HIS:O	2.19	0.42
1:E:18:HIS:CE1	6:E:221:HOH:O	2.73	0.42
1:F:177:VAL:O	1:F:180:LYS:HB3	2.19	0.42
2:Q:438:SER:O	4:Q:601:BME:H22	2.20	0.42
2:O:361:HIS:HD2	6:O:711:HOH:O	2.02	0.42
1:E:19:ILE:HG21	1:E:19:ILE:HD13	1.76	0.42
2:R:489:CYS:O	2:R:493:LYS:HE3	2.19	0.42
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.78	0.42
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.34	0.42
2:R:372:LEU:HA	2:R:373:PRO:HD3	1.84	0.42
2:P:443:LYS:HA	2:P:444:PRO:HD2	1.94	0.42
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.35	0.42
2:M:390:LYS:HA	2:M:391:PRO:HD3	1.88	0.42
1:F:116:ASN:C	1:F:116:ASN:OD1	2.58	0.42
1:F:176:GLU:HG3	1:F:180:LYS:C	2.39	0.41
1:F:18:HIS:CE1	6:F:1278:HOH:O	2.72	0.41
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.54	0.41
1:E:9:PRO:HD2	2:Q:504:LEU:HD21	2.01	0.41
2:R:392:VAL:HG12	2:R:395:THR:HB	2.02	0.41
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.41
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.19	0.41
2:N:497:ASN:HD22	2:N:497:ASN:C	2.23	0.41
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.79	0.41
2:O:390:LYS:HD3	6:O:732:HOH:O	2.20	0.41
2:P:390:LYS:HA	2:P:391:PRO:HD3	1.88	0.41
1:E:100:ASP:CG	1:E:101:ALA:H	2.23	0.41
1:D:51:LEU:HD12	1:D:106:LEU:HD23	2.03	0.41
2:Q:360:ASP:HB3	2:Q:428:ARG:HG3	2.01	0.41
2:Q:495:ILE:HG21	2:Q:500:ALA:HB3	2.02	0.41
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.82	0.41
2:M:473:LYS:NZ	6:M:651:HOH:O	2.44	0.41
1:B:44:ALA:HA	1:B:45:PRO:HD2	1.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.56	0.41
2:N:392:VAL:HG12	2:N:395:THR:HB	2.02	0.41
1:E:24:GLU:O	1:E:27:GLY:N	2.50	0.41
2:O:416:LEU:CD2	2:O:416:LEU:C	2.87	0.41
2:M:447:TYR:HB2	2:M:448:PRO:HD2	2.02	0.41
2:Q:304:ASP:HB2	2:Q:343:ILE:HB	2.02	0.41
1:C:5:LEU:O	2:O:387:GLN:HG2	2.20	0.41
1:D:98:THR:OG1	1:D:101:ALA:HB3	2.20	0.41
2:P:522:ARG:NH1	6:P:673:HOH:O	2.24	0.41
2:M:488:MET:CE	2:P:508:LEU:HD23	2.50	0.41
2:O:450:ARG:HG3	6:O:642:HOH:O	2.21	0.41
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.21	0.41
1:C:180:LYS:HG2	1:C:181:THR:N	2.36	0.41
1:D:51:LEU:O	1:D:52:LEU:HB3	2.21	0.41
1:B:143:LEU:C	1:B:143:LEU:HD23	2.41	0.41
2:M:335:ALA:HB2	2:O:328:ILE:HD12	2.02	0.41
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.74	0.41
2:M:326:THR:HG22	2:M:330:ARG:HD2	2.03	0.41
1:D:18:HIS:HA	1:D:22:ALA:HB3	2.03	0.41
1:A:70:VAL:HA	1:A:127:ASN:O	2.21	0.41
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.39	0.40
2:Q:392:VAL:HG12	2:Q:395:THR:HB	2.03	0.40
2:P:405:GLY:HA3	6:P:653:HOH:O	2.20	0.40
2:M:399:MET:HA	2:M:462:HIS:O	2.21	0.40
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.80	0.40
1:B:100:ASP:CG	1:B:101:ALA:H	2.24	0.40
1:A:39:LEU:HD11	1:A:93:GLY:HA3	2.02	0.40
1:D:35:ILE:HD13	2:P:351:PHE:CE1	2.56	0.40
2:R:407:ARG:HG2	2:R:407:ARG:NH1	2.37	0.40
1:E:157:VAL:O	1:E:160:LEU:HB2	2.21	0.40
2:P:457:ARG:HA	2:P:458:PRO:HD3	1.90	0.40
1:D:19:ILE:O	2:P:426:VAL:HG21	2.20	0.40
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.87	0.40
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.40	0.40
1:D:24:GLU:O	1:D:27:GLY:CA	2.69	0.40
1:F:52:LEU:HD22	1:F:52:LEU:C	2.42	0.40
2:P:443:LYS:HE2	2:P:480:PHE:CG	2.57	0.40
2:N:449:TRP:CD1	2:N:449:TRP:N	2.89	0.40
2:N:447:TYR:HB2	2:N:448:PRO:HD2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:GLN:NE2	6:C:275:HOH:O[3_445]	1.36	0.84
1:C:46:GLY:O	1:D:150:GLN:OE1[3_554]	1.84	0.36
6:Q:1200:HOH:O	6:Q:1200:HOH:O[2_555]	2.10	0.10

## 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%)	193 (98%)	5 (2%)	0	100	100
1	F	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
2	M	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	N	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	Q	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
2	R	229/238 (96%)	221 (96%)	7 (3%)	1 (0%)	43	45
All	All	2562/2628 (98%)	2475 (97%)	86 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	535	PHE

### 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%)	156 (96%)	6 (4%)	45	54
1	B	162/163 (99%)	155 (96%)	7 (4%)	40	46
1	C	162/163 (99%)	155 (96%)	7 (4%)	40	46
1	D	162/163 (99%)	155 (96%)	7 (4%)	40	46
1	E	162/163 (99%)	155 (96%)	7 (4%)	40	46
1	F	162/163 (99%)	155 (96%)	7 (4%)	40	46
2	M	196/202 (97%)	188 (96%)	8 (4%)	41	49
2	N	196/202 (97%)	183 (93%)	13 (7%)	24	24
2	O	196/202 (97%)	186 (95%)	10 (5%)	33	37
2	P	196/202 (97%)	189 (96%)	7 (4%)	47	56
2	Q	196/202 (97%)	185 (94%)	11 (6%)	30	32
2	R	196/202 (97%)	185 (94%)	11 (6%)	30	32
All	All	2148/2190 (98%)	2047 (95%)	101 (5%)	36	42

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	91	SER
1	A	165	GLN
2	M	344	SER
2	M	395	THR
2	M	416	LEU
2	M	434	ASP
2	M	440	ARG
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	38	ARG
1	B	52	LEU
1	B	106	LEU
1	B	158	LEU

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Mol	Chain	Res	Type
1	B	165	GLN
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	411	LYS
2	N	416	LEU
2	N	428	ARG
2	N	433	SER
2	N	440	ARG
2	N	442	ILE
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	100	ASP
1	C	158	LEU
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	434	ASP
2	O	465	ILE
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS
1	D	4	LEU
1	D	19	ILE
1	D	38	ARG
1	D	42	PRO
1	D	43	ASP
1	D	52	LEU
1	D	165	GLN
2	P	364	LEU
2	P	395	THR
2	P	411	LYS
2	P	416	LEU

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Mol	Chain	Res	Type
2	P	440	ARG
2	P	497	ASN
2	P	534	HIS
1	E	4	LEU
1	E	38	ARG
1	E	49	ILE
1	E	52	LEU
1	E	66	SER
1	E	165	GLN
1	E	181	THR
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	411	LYS
2	Q	416	LEU
2	Q	428	ARG
2	Q	442	ILE
2	Q	450	ARG
2	Q	478	LEU
2	Q	497	ASN
2	Q	507	LYS
1	F	4	LEU
1	F	30	THR
1	F	50	LEU
1	F	52	LEU
1	F	66	SER
1	F	100	ASP
1	F	165	GLN
2	R	352	SER
2	R	372	LEU
2	R	395	THR
2	R	399	MET
2	R	411	LYS
2	R	416	LEU
2	R	428	ARG
2	R	440	ARG
2	R	442	ILE
2	R	497	ASN
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	165	GLN
2	N	361	HIS
2	N	497	ASN
2	N	503	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	163	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	107	HIS
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	422	ASN
2	R	497	ASN
2	R	503	GLN
2	R	530	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	IHB	M	550	3	11,11,11	1.48	2 (18%)	15,15,15	0.40	0
5	IHB	M	551	-	11,11,11	1.38	2 (18%)	15,15,15	0.94	1 (6%)
4	BME	M	601	2	3,3,3	0.53	0	2,2,2	0.11	0
5	IHB	N	550	3	11,11,11	1.55	2 (18%)	15,15,15	0.69	0
5	IHB	N	551	-	11,11,11	1.36	2 (18%)	15,15,15	0.92	1 (6%)
4	BME	N	601	2	3,3,3	0.44	0	2,2,2	0.39	0
5	IHB	O	550	3	11,11,11	1.37	2 (18%)	15,15,15	0.36	0
5	IHB	O	551	-	11,11,11	1.33	2 (18%)	15,15,15	1.05	2 (13%)
4	BME	O	601	2	3,3,3	0.62	0	2,2,2	1.04	0
5	IHB	P	550	3	11,11,11	1.33	2 (18%)	15,15,15	0.60	0
5	IHB	P	551	-	11,11,11	1.46	3 (27%)	15,15,15	1.03	2 (13%)
4	BME	P	601	2	3,3,3	0.57	0	2,2,2	1.21	0
5	IHB	Q	550	3	11,11,11	1.44	2 (18%)	15,15,15	0.51	0
5	IHB	Q	551	-	11,11,11	1.23	2 (18%)	15,15,15	0.73	1 (6%)
4	BME	Q	601	2	3,3,3	0.41	0	2,2,2	1.90	1 (50%)
5	IHB	R	550	3	11,11,11	1.36	2 (18%)	15,15,15	0.47	0
5	IHB	R	551	-	11,11,11	1.22	2 (18%)	15,15,15	1.09	1 (6%)
4	BME	R	601	2	3,3,3	0.54	0	2,2,2	1.11	0

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

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	IHB	C1-C7	3.70	1.56	1.49
5	O	550	IHB	C1-C7	3.35	1.56	1.49
5	Q	550	IHB	C1-C7	3.29	1.55	1.49
5	M	550	IHB	C1-C7	3.05	1.55	1.49
5	M	550	IHB	C3-I3	-2.97	2.01	2.10
5	N	551	IHB	C1-C7	2.93	1.55	1.49
5	R	550	IHB	C3-I3	-2.79	2.01	2.10
5	P	550	IHB	C1-C7	2.76	1.54	1.49
5	O	551	IHB	C3-I3	-2.75	2.01	2.10
5	P	551	IHB	C1-C7	2.70	1.54	1.49
5	N	550	IHB	C3-I3	-2.61	2.02	2.10
5	M	551	IHB	C1-C7	2.60	1.54	1.49
5	P	551	IHB	C3-I3	-2.52	2.02	2.10
5	R	550	IHB	C1-C7	2.51	1.54	1.49
5	Q	550	IHB	C3-I3	-2.51	2.02	2.10
5	M	551	IHB	C3-I3	-2.49	2.02	2.10
5	N	551	IHB	O2-C7	-2.49	1.22	1.30
5	Q	551	IHB	C1-C7	2.48	1.54	1.49
5	P	550	IHB	C3-I3	-2.46	2.02	2.10
5	R	551	IHB	C1-C7	2.23	1.53	1.49
5	O	551	IHB	C1-C7	2.20	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	551	IHB	O2-C7	-2.20	1.23	1.30
5	R	551	IHB	C3-I3	-2.18	2.03	2.10
5	O	550	IHB	C3-I3	-2.14	2.03	2.10
5	Q	551	IHB	O2-C7	-2.08	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	601	BME	C1-C2-S2	-2.69	108.40	113.03
5	N	551	IHB	O2-C7-O1	-2.65	117.34	123.35
5	P	551	IHB	O2-C7-O1	-2.48	117.73	123.35
5	M	551	IHB	O2-C7-C1	2.38	121.30	115.01
5	P	551	IHB	O2-C7-C1	2.33	121.18	115.01
5	O	551	IHB	O2-C7-O1	-2.29	118.16	123.35
5	R	551	IHB	O2-C7-C1	2.29	121.06	115.01
5	O	551	IHB	O2-C7-C1	2.15	120.69	115.01
5	Q	551	IHB	O2-C7-O1	-2.05	118.70	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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