



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:34 PM GMT

PDB ID : 1RSC  
Title : STRUCTURE OF AN EFFECTOR INDUCED INACTIVATED STATE OF  
RIBULOSE BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE  
:THE BINARY COMPLEX BETWEEN ENZYME AND XYLULOSE BIS-  
PHOSPHATE  
Authors : Newman, J.; Gutteridge, S.  
Deposited on : 1994-03-29  
Resolution : 2.30 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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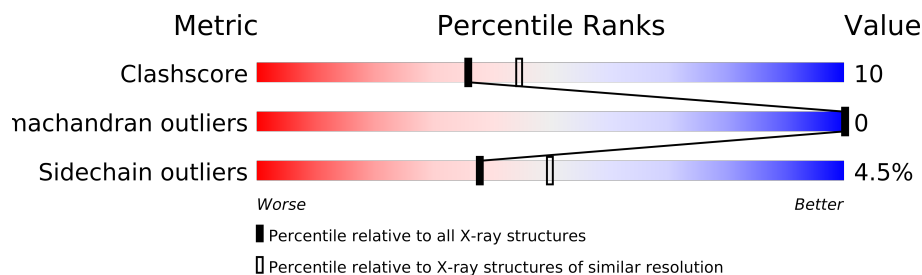
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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	472	
1	B	472	
1	C	472	
1	D	472	
1	E	472	
1	F	472	
1	G	472	
1	H	472	
2	I	111	
2	J	111	
2	K	111	
2	L	111	
2	M	111	
2	N	111	
2	O	111	
2	P	111	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36846 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 RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYG ENASE(LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	B	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	C	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	D	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	E	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	F	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	G	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			
1	H	467	Total	C	N	O	S	72	0	0
			3653	2324	638	673	18			

- Molecule 2 is a protein called RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYG ENASE(SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	I	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	N	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	J	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	O	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			

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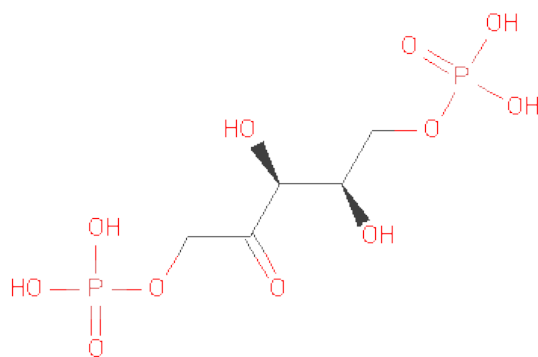
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	P	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	L	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	109	GLU	GLN	CONFLICT	UNP P04716
I	109	GLU	GLN	CONFLICT	UNP P04716
N	109	GLU	GLN	CONFLICT	UNP P04716
J	109	GLU	GLN	CONFLICT	UNP P04716
O	109	GLU	GLN	CONFLICT	UNP P04716
K	109	GLU	GLN	CONFLICT	UNP P04716
P	109	GLU	GLN	CONFLICT	UNP P04716
L	109	GLU	GLN	CONFLICT	UNP P04716

- Molecule 3 is SUGAR (XYLULOSE-1,5-BISPHOSPHATE) (three-letter code: XBP) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			18	5	11	2		
3	B	1	Total	C	O	P	0	0
			18	5	11	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 18	C 5	O 11	P 2	0	0
3	D	1	Total 18	C 5	O 11	P 2	0	0
3	E	1	Total 18	C 5	O 11	P 2	0	0
3	F	1	Total 18	C 5	O 11	P 2	0	0
3	G	1	Total 18	C 5	O 11	P 2	0	0
3	H	1	Total 18	C 5	O 11	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	148	Total 148	O 148	0	0
4	B	9	Total 9	O 9	0	0
4	C	8	Total 8	O 8	0	0
4	D	4	Total 4	O 4	0	0
4	G	1	Total 1	O 1	0	0
4	J	1	Total 1	O 1	0	0
4	M	35	Total 35	O 35	0	0

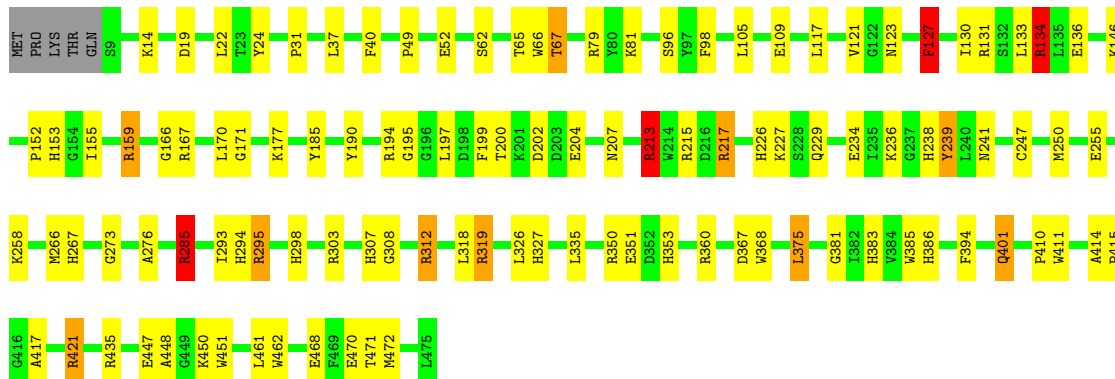
### 3 Residue-property plots

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.

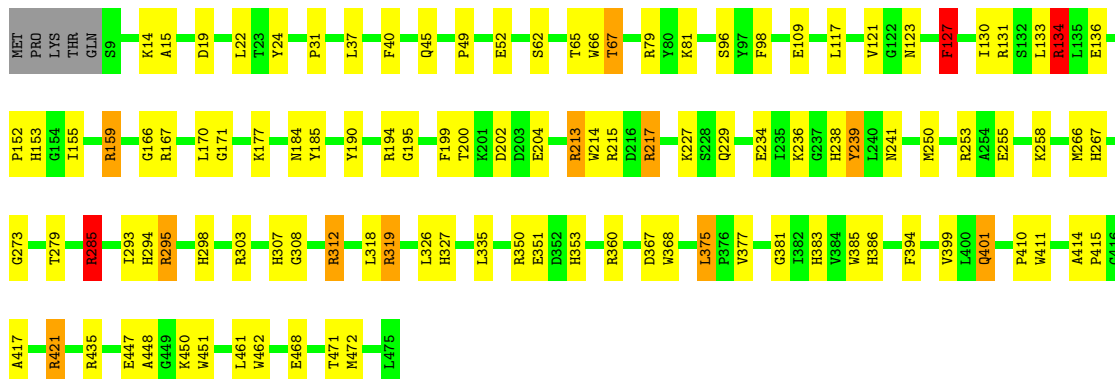
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain A: 



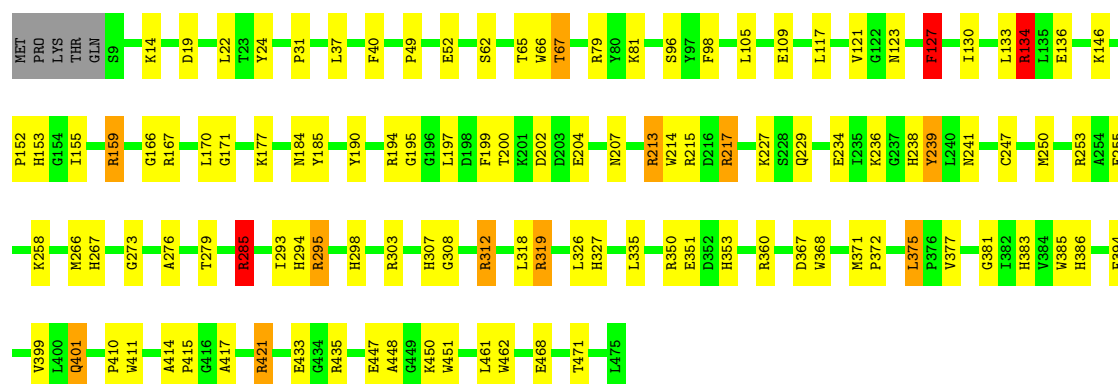
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain B: 



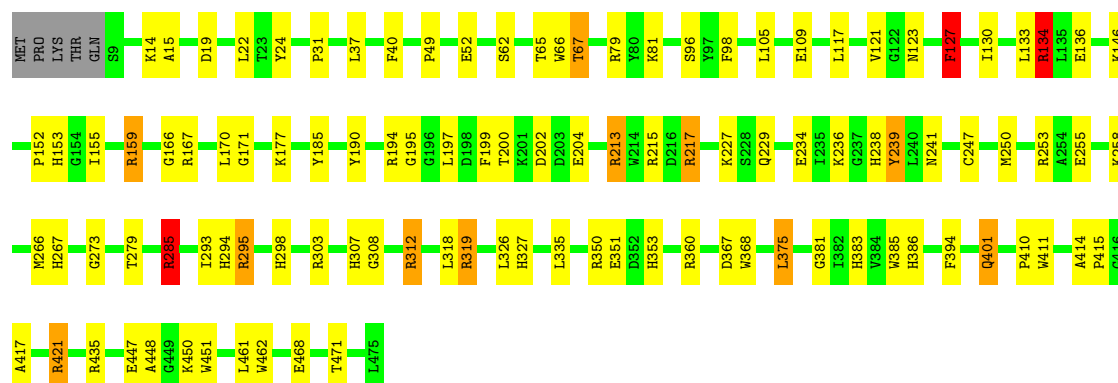
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain C: 



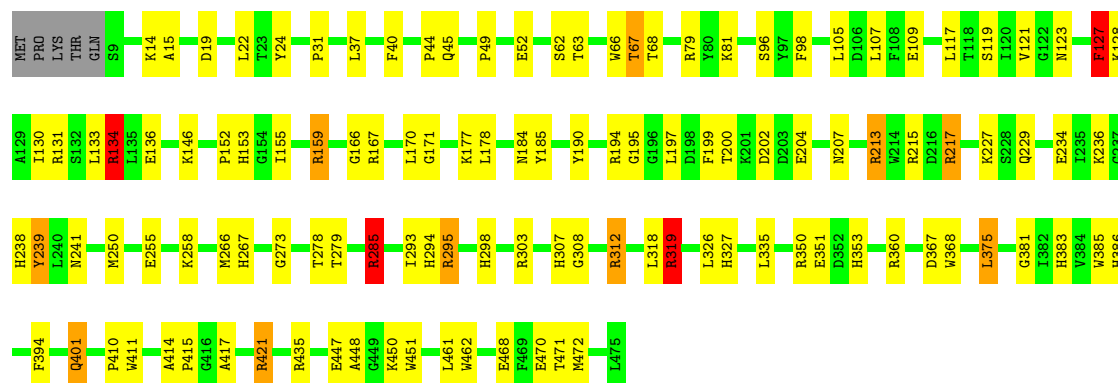
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain D:



• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

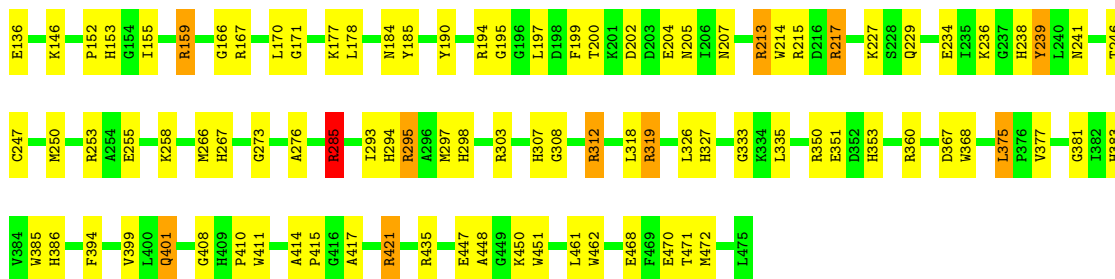
Chain E:



• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

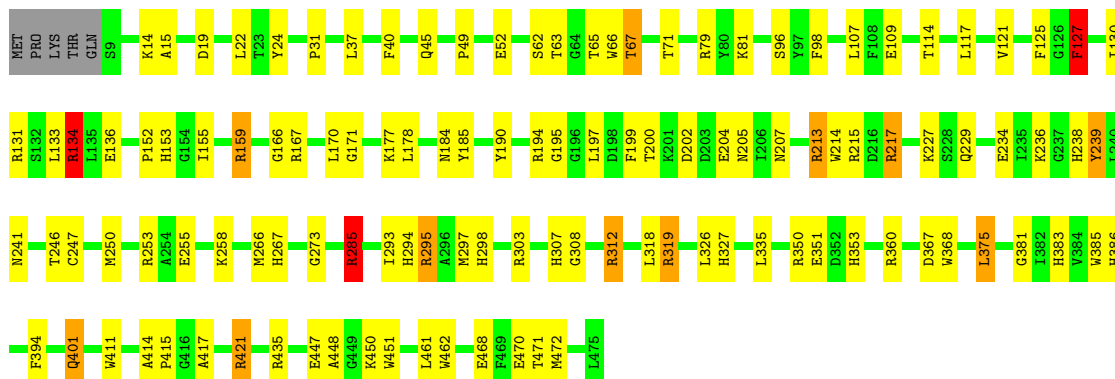
Chain F:





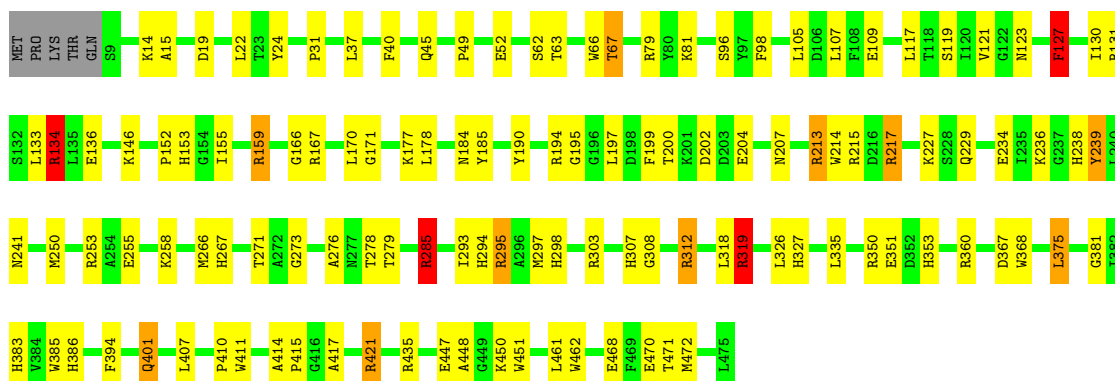
- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain G:



- Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(LARGE CHAIN)

Chain H:



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain M:



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain I: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain N: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain J: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain O: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain K: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain P: 



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE(SMALL CHAIN)

Chain L: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.40Å 112.60Å 200.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.255 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: XBP

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	0.32	1/3745 (0.0%)	0.51	1/5071 (0.0%)
1	B	0.32	1/3745 (0.0%)	0.51	1/5071 (0.0%)
1	C	0.32	1/3745 (0.0%)	0.52	1/5071 (0.0%)
1	D	0.32	1/3745 (0.0%)	0.51	1/5071 (0.0%)
1	E	0.32	1/3745 (0.0%)	0.52	1/5071 (0.0%)
1	F	0.32	1/3745 (0.0%)	0.52	1/5071 (0.0%)
1	G	0.32	1/3745 (0.0%)	0.52	1/5071 (0.0%)
1	H	0.32	1/3745 (0.0%)	0.51	1/5071 (0.0%)
2	I	0.30	0/936	0.46	0/1267
2	J	0.30	0/936	0.46	0/1267
2	K	0.30	0/936	0.46	0/1267
2	L	0.30	0/936	0.46	0/1267
2	M	0.30	0/936	0.46	0/1267
2	N	0.30	0/936	0.46	0/1267
2	O	0.30	0/936	0.47	0/1267
2	P	0.31	0/936	0.47	0/1267
All	All	0.32	8/37448 (0.0%)	0.51	8/50704 (0.0%)

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	A	0	9
1	B	0	9
1	C	0	9
1	D	0	9
1	E	0	9
1	F	0	9
1	G	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	9
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	1
2	M	0	1
2	N	0	1
2	O	0	1
2	P	0	1
All	All	0	80

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	127	PHE	CA-CB	-6.84	1.39	1.53
1	H	127	PHE	CA-CB	-6.76	1.39	1.53
1	C	127	PHE	CA-CB	-6.76	1.39	1.53
1	A	127	PHE	CA-CB	-6.75	1.39	1.53
1	B	127	PHE	CA-CB	-6.75	1.39	1.53
1	D	127	PHE	CA-CB	-6.75	1.39	1.53
1	F	127	PHE	CA-CB	-6.74	1.39	1.53
1	E	127	PHE	CA-CB	-6.70	1.39	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	217	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	217	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	217	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	E	217	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	H	217	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	217	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	F	217	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	G	217	ARG	NE-CZ-NH2	-5.38	117.61	120.30

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	159	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	194	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	217	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	312	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	421	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	194	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	312	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	421	ARG	Sidechain
1	C	134	ARG	Sidechain
1	C	159	ARG	Sidechain
1	C	194	ARG	Sidechain
1	C	213	ARG	Sidechain
1	C	217	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	421	ARG	Sidechain
1	D	134	ARG	Sidechain
1	D	159	ARG	Sidechain
1	D	194	ARG	Sidechain
1	D	213	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	312	ARG	Sidechain
1	D	319	ARG	Sidechain
1	D	421	ARG	Sidechain
1	E	134	ARG	Sidechain
1	E	159	ARG	Sidechain
1	E	194	ARG	Sidechain
1	E	213	ARG	Sidechain
1	E	217	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	312	ARG	Sidechain
1	E	319	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	421	ARG	Sidechain
1	F	134	ARG	Sidechain
1	F	159	ARG	Sidechain
1	F	194	ARG	Sidechain
1	F	213	ARG	Sidechain
1	F	217	ARG	Sidechain
1	F	285	ARG	Sidechain
1	F	312	ARG	Sidechain
1	F	319	ARG	Sidechain
1	F	421	ARG	Sidechain
1	G	134	ARG	Sidechain
1	G	159	ARG	Sidechain
1	G	194	ARG	Sidechain
1	G	213	ARG	Sidechain
1	G	217	ARG	Sidechain
1	G	285	ARG	Sidechain
1	G	312	ARG	Sidechain
1	G	319	ARG	Sidechain
1	G	421	ARG	Sidechain
1	H	134	ARG	Sidechain
1	H	159	ARG	Sidechain
1	H	194	ARG	Sidechain
1	H	213	ARG	Sidechain
1	H	217	ARG	Sidechain
1	H	285	ARG	Sidechain
1	H	312	ARG	Sidechain
1	H	319	ARG	Sidechain
1	H	421	ARG	Sidechain
2	I	66	TYR	Sidechain
2	J	66	TYR	Sidechain
2	K	66	TYR	Sidechain
2	L	66	TYR	Sidechain
2	M	66	TYR	Sidechain
2	N	66	TYR	Sidechain
2	O	66	TYR	Sidechain
2	P	66	TYR	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	3653	0	3568	93	0
1	B	3653	0	3568	90	0
1	C	3653	0	3568	88	1
1	D	3653	0	3568	82	0
1	E	3653	0	3568	102	0
1	F	3653	0	3568	105	0
1	G	3653	0	3568	113	0
1	H	3653	0	3568	117	0
2	I	909	0	860	14	1
2	J	909	0	860	15	1
2	K	909	0	860	11	30
2	L	909	0	860	14	0
2	M	909	0	860	16	1
2	N	909	0	860	13	0
2	O	909	0	860	16	30
2	P	909	0	860	16	0
3	A	18	0	8	2	0
3	B	18	0	8	2	0
3	C	18	0	8	2	0
3	D	18	0	8	2	0
3	E	18	0	8	2	0
3	F	18	0	8	1	0
3	G	18	0	8	1	0
3	H	18	0	8	2	0
4	A	148	0	0	3	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	4	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
4	M	35	0	0	1	0
All	All	36846	0	35488	721	32

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 10.

All (721) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:462:TRP:HE1	1:H:67:THR:HG21	1.07	1.17

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:462:TRP:HE1	1:F:67:THR:HG21	0.98	1.14
1:C:462:TRP:HE1	1:D:67:THR:HG21	1.12	1.14
1:G:67:THR:HG21	1:H:462:TRP:HE1	1.02	1.11
1:A:462:TRP:HE1	1:B:67:THR:HG21	1.01	1.09
1:E:67:THR:HG21	1:F:462:TRP:HE1	1.02	1.09
1:A:67:THR:HG21	1:B:462:TRP:HE1	1.11	1.09
1:C:67:THR:HG21	1:D:462:TRP:HE1	1.15	1.05
1:H:295:ARG:HD3	3:H:476:XBP:O4P	1.60	1.01
1:F:295:ARG:HD3	3:F:476:XBP:O4P	1.61	1.01
1:G:295:ARG:HD3	3:G:476:XBP:O4P	1.60	1.01
1:D:295:ARG:HD3	3:D:476:XBP:O4P	1.60	1.01
1:B:295:ARG:HD3	3:B:476:XBP:O4P	1.60	1.00
1:E:295:ARG:HD3	3:E:476:XBP:O4P	1.61	1.00
1:C:295:ARG:HD3	3:C:476:XBP:O4P	1.60	1.00
1:G:67:THR:HG21	1:H:462:TRP:NE1	1.75	1.00
1:A:295:ARG:HD3	3:A:476:XBP:O4P	1.60	0.99
1:E:462:TRP:NE1	1:F:67:THR:HG21	1.76	0.99
1:E:67:THR:HG21	1:F:462:TRP:NE1	1.79	0.98
1:G:462:TRP:NE1	1:H:67:THR:HG21	1.79	0.98
1:A:462:TRP:NE1	1:B:67:THR:HG21	1.78	0.96
1:C:462:TRP:NE1	1:D:67:THR:HG21	1.90	0.87
1:A:67:THR:HG21	1:B:462:TRP:NE1	1.89	0.86
1:G:335:LEU:CD2	1:H:127:PHE:CD1	2.62	0.83
1:C:250:MET:CE	1:C:267:HIS:NE2	2.44	0.81
1:F:250:MET:CE	1:F:267:HIS:NE2	2.44	0.81
1:E:250:MET:CE	1:E:267:HIS:NE2	2.44	0.81
1:E:67:THR:CG2	1:F:462:TRP:HE1	1.91	0.80
1:A:250:MET:CE	1:A:267:HIS:NE2	2.44	0.80
1:H:250:MET:CE	1:H:267:HIS:NE2	2.44	0.80
1:B:250:MET:CE	1:B:267:HIS:NE2	2.44	0.80
1:G:250:MET:CE	1:G:267:HIS:NE2	2.44	0.80
1:D:250:MET:CE	1:D:267:HIS:NE2	2.44	0.80
1:C:67:THR:HG21	1:D:462:TRP:NE1	1.94	0.79
1:G:66:TRP:CD1	1:H:381:GLY:HA2	2.20	0.76
2:O:41:LEU:HD11	2:O:69:MET:HG3	1.69	0.74
2:L:41:LEU:HD11	2:L:69:MET:HG3	1.69	0.74
2:J:41:LEU:HD11	2:J:69:MET:HG3	1.69	0.74
2:N:41:LEU:HD11	2:N:69:MET:HG3	1.69	0.74
2:I:41:LEU:HD11	2:I:69:MET:HG3	1.69	0.73
2:K:41:LEU:HD11	2:K:69:MET:HG3	1.69	0.73
2:M:41:LEU:HD11	2:M:69:MET:HG3	1.69	0.73
1:D:250:MET:HE2	1:D:267:HIS:NE2	2.05	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:41:LEU:HD11	2:P:69:MET:HG3	1.70	0.72
1:H:250:MET:HE2	1:H:267:HIS:NE2	2.05	0.72
1:G:15:ALA:HB1	1:H:461:LEU:HD21	1.71	0.72
1:E:250:MET:HE2	1:E:267:HIS:NE2	2.04	0.71
1:B:250:MET:HE2	1:B:267:HIS:NE2	2.04	0.71
1:E:127:PHE:CD1	1:F:335:LEU:CD2	2.73	0.71
1:G:335:LEU:HD21	1:H:127:PHE:CD1	2.24	0.70
1:E:462:TRP:HE1	1:F:67:THR:CG2	1.91	0.70
1:G:127:PHE:CD1	1:H:335:LEU:CD2	2.73	0.70
1:F:250:MET:HE2	1:F:267:HIS:NE2	2.06	0.69
1:G:250:MET:HE2	1:G:267:HIS:NE2	2.05	0.69
1:C:250:MET:HE2	1:C:267:HIS:NE2	2.06	0.69
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.75	0.69
1:G:303:ARG:NH2	1:H:130:ILE:O	2.26	0.69
1:G:335:LEU:HD23	1:H:127:PHE:CD1	2.26	0.69
1:A:250:MET:HE1	1:A:267:HIS:CE1	2.28	0.69
1:F:234:GLU:OE1	1:F:421:ARG:NH2	2.27	0.68
1:D:234:GLU:OE1	1:D:421:ARG:NH2	2.27	0.68
1:A:462:TRP:HE1	1:B:67:THR:CG2	1.93	0.68
1:G:127:PHE:CD1	1:H:335:LEU:HD23	2.28	0.68
1:G:234:GLU:OE1	1:G:421:ARG:NH2	2.27	0.68
1:G:253:ARG:NH2	1:H:109:GLU:OE2	2.20	0.68
1:G:462:TRP:HE1	1:H:67:THR:CG2	1.96	0.68
1:A:234:GLU:OE1	1:A:421:ARG:NH2	2.27	0.67
1:C:234:GLU:OE1	1:C:421:ARG:NH2	2.27	0.67
1:H:234:GLU:OE1	1:H:421:ARG:NH2	2.27	0.67
1:E:234:GLU:OE1	1:E:421:ARG:NH2	2.27	0.67
1:G:273:GLY:HA3	1:H:273:GLY:HA3	1.76	0.67
1:E:383:HIS:H	1:E:386:HIS:HD2	1.44	0.66
1:E:127:PHE:CD1	1:F:335:LEU:HD21	2.31	0.66
1:B:234:GLU:OE1	1:B:421:ARG:NH2	2.27	0.66
1:D:383:HIS:H	1:D:386:HIS:HD2	1.44	0.66
1:A:383:HIS:H	1:A:386:HIS:HD2	1.44	0.66
1:C:383:HIS:H	1:C:386:HIS:HD2	1.44	0.65
1:B:383:HIS:H	1:B:386:HIS:HD2	1.44	0.65
1:G:383:HIS:H	1:G:386:HIS:HD2	1.44	0.65
1:A:155:ILE:HG12	1:A:375:LEU:HD13	1.79	0.65
1:E:155:ILE:HG12	1:E:375:LEU:HD13	1.79	0.65
1:D:155:ILE:HG12	1:D:375:LEU:HD13	1.78	0.65
1:H:383:HIS:H	1:H:386:HIS:HD2	1.44	0.65
2:P:30:ILE:O	2:P:34:ILE:HG12	1.97	0.65
1:H:155:ILE:HG12	1:H:375:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:155:ILE:HG12	1:G:375:LEU:HD13	1.78	0.65
1:F:383:HIS:H	1:F:386:HIS:HD2	1.44	0.65
2:J:30:ILE:O	2:J:34:ILE:HG12	1.97	0.65
1:B:155:ILE:HG12	1:B:375:LEU:HD13	1.78	0.64
2:I:30:ILE:O	2:I:34:ILE:HG12	1.97	0.64
1:G:335:LEU:CD2	1:H:127:PHE:HD1	2.10	0.64
2:M:30:ILE:O	2:M:34:ILE:HG12	1.97	0.64
1:C:155:ILE:HG12	1:C:375:LEU:HD13	1.79	0.64
2:L:30:ILE:O	2:L:34:ILE:HG12	1.97	0.64
2:N:30:ILE:O	2:N:34:ILE:HG12	1.97	0.64
1:F:155:ILE:HG12	1:F:375:LEU:HD13	1.79	0.64
2:K:30:ILE:O	2:K:34:ILE:HG12	1.97	0.63
1:E:335:LEU:CD2	1:F:127:PHE:CD1	2.81	0.63
1:G:381:GLY:HA2	1:H:66:TRP:CD1	2.33	0.63
1:A:335:LEU:CD2	1:B:127:PHE:CD1	2.82	0.63
2:O:30:ILE:O	2:O:34:ILE:HG12	1.98	0.63
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.80	0.61
1:E:350:ARG:NH2	1:E:394:PHE:O	2.34	0.61
1:H:350:ARG:NH2	1:H:394:PHE:O	2.34	0.61
1:A:127:PHE:CD1	1:B:335:LEU:CD2	2.83	0.61
1:F:350:ARG:NH2	1:F:394:PHE:O	2.34	0.61
1:G:350:ARG:NH2	1:G:394:PHE:O	2.34	0.61
1:A:350:ARG:NH2	1:A:394:PHE:O	2.34	0.61
1:C:350:ARG:NH2	1:C:394:PHE:O	2.34	0.60
1:G:66:TRP:CH2	1:H:383:HIS:HD2	2.18	0.60
1:C:273:GLY:HA3	1:D:273:GLY:HA3	1.83	0.60
1:E:127:PHE:CD1	1:F:335:LEU:HD23	2.37	0.60
1:B:350:ARG:NH2	1:B:394:PHE:O	2.34	0.60
1:A:250:MET:HE1	1:A:267:HIS:NE2	2.16	0.59
1:D:350:ARG:NH2	1:D:394:PHE:O	2.34	0.59
3:E:476:XBP:O2P	1:F:65:THR:OG1	2.15	0.59
1:E:130:ILE:O	1:F:303:ARG:NH2	2.34	0.59
1:G:461:LEU:HD21	1:H:15:ALA:HB1	1.85	0.59
1:G:177:LYS:HB2	1:H:63:THR:HA	1.85	0.58
1:A:65:THR:OG1	3:B:476:XBP:O2P	2.17	0.58
1:G:107:LEU:HD22	1:H:178:LEU:HD12	1.85	0.58
1:G:107:LEU:HD22	1:H:178:LEU:CD1	2.34	0.58
1:G:470:GLU:O	1:H:45:GLN:NE2	2.37	0.58
1:G:130:ILE:O	1:H:303:ARG:NH2	2.36	0.58
1:G:131:ARG:O	1:H:472:MET:HG3	2.04	0.58
1:G:178:LEU:CD1	1:H:107:LEU:HD22	2.34	0.58
1:G:319:ARG:NH2	1:G:351:GLU:O	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:297:MET:HA	1:H:121:VAL:O	2.05	0.57
1:C:319:ARG:NH2	1:C:351:GLU:O	2.35	0.57
1:B:229:GLN:NE2	1:B:236:LYS:H	2.03	0.57
1:E:229:GLN:NE2	1:E:236:LYS:H	2.03	0.56
1:C:229:GLN:NE2	1:C:236:LYS:H	2.03	0.56
1:A:229:GLN:NE2	1:A:236:LYS:H	2.03	0.56
1:B:411:TRP:CD1	2:I:3:MET:HB3	2.41	0.56
1:E:234:GLU:CD	1:E:421:ARG:HH22	2.09	0.56
1:E:335:LEU:HD23	1:F:127:PHE:CD1	2.39	0.56
1:H:411:TRP:CD1	2:L:3:MET:HB3	2.41	0.56
1:D:411:TRP:CD1	2:J:3:MET:HB3	2.41	0.56
1:D:318:LEU:O	1:D:318:LEU:HG	2.06	0.56
1:C:335:LEU:CD2	1:D:127:PHE:CD1	2.89	0.56
1:D:229:GLN:NE2	1:D:236:LYS:H	2.03	0.56
1:F:229:GLN:NE2	1:F:236:LYS:H	2.03	0.56
1:C:234:GLU:CD	1:C:421:ARG:HH22	2.09	0.56
1:F:411:TRP:CD1	2:K:3:MET:HB3	2.41	0.56
1:E:411:TRP:CD1	2:O:3:MET:HB3	2.41	0.56
1:H:229:GLN:NE2	1:H:236:LYS:H	2.03	0.56
1:C:411:TRP:CD1	2:N:3:MET:HB3	2.41	0.56
1:E:123:ASN:ND2	1:F:204:GLU:OE2	2.38	0.56
1:G:229:GLN:NE2	1:G:236:LYS:H	2.03	0.56
1:A:319:ARG:NH2	1:A:351:GLU:O	2.35	0.56
1:H:234:GLU:CD	1:H:421:ARG:HH22	2.10	0.56
1:C:127:PHE:CD1	1:D:335:LEU:CD2	2.89	0.56
1:B:318:LEU:HG	1:B:318:LEU:O	2.06	0.56
1:A:250:MET:HE2	1:A:267:HIS:NE2	2.21	0.55
1:E:127:PHE:HD1	1:F:335:LEU:CD2	2.17	0.55
1:C:318:LEU:O	1:C:318:LEU:HG	2.06	0.55
1:B:234:GLU:CD	1:B:421:ARG:HH22	2.10	0.55
3:A:476:XBP:O2P	1:B:65:THR:OG1	2.15	0.55
1:E:381:GLY:HA2	1:F:66:TRP:CD1	2.40	0.55
1:A:123:ASN:ND2	1:B:204:GLU:OE2	2.39	0.55
1:G:45:GLN:NE2	1:H:470:GLU:O	2.40	0.55
1:A:411:TRP:CD1	2:M:3:MET:HB3	2.41	0.55
1:F:318:LEU:O	1:F:318:LEU:HG	2.06	0.55
1:A:335:LEU:HD23	1:B:127:PHE:CD1	2.42	0.55
1:A:127:PHE:CD1	1:B:335:LEU:HD21	2.42	0.55
1:G:411:TRP:CD1	2:P:3:MET:HB3	2.41	0.55
1:F:234:GLU:CD	1:F:421:ARG:HH22	2.10	0.55
1:B:319:ARG:NH2	1:B:351:GLU:O	2.35	0.55
1:A:318:LEU:HG	1:A:318:LEU:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:127:PHE:CD1	1:H:335:LEU:HD21	2.42	0.55
1:D:234:GLU:CD	1:D:421:ARG:HH22	2.10	0.55
1:H:318:LEU:O	1:H:318:LEU:HG	2.06	0.55
1:E:62:SER:O	1:F:177:LYS:HB2	2.07	0.55
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.42	0.54
1:G:67:THR:CG2	1:H:462:TRP:HE1	1.95	0.54
1:D:250:MET:HE2	1:D:267:HIS:CD2	2.43	0.54
1:D:319:ARG:NH2	1:D:351:GLU:O	2.35	0.54
1:E:472:MET:HG3	1:F:131:ARG:O	2.07	0.54
1:G:15:ALA:HB1	1:H:461:LEU:CD2	2.37	0.54
1:E:250:MET:CE	1:E:267:HIS:CE1	2.91	0.54
1:A:234:GLU:CD	1:A:421:ARG:HH22	2.09	0.54
1:G:472:MET:HG3	1:H:131:ARG:O	2.07	0.54
1:G:318:LEU:HG	1:G:318:LEU:O	2.06	0.54
1:G:234:GLU:CD	1:G:421:ARG:HH22	2.10	0.54
1:F:319:ARG:NH2	1:F:351:GLU:O	2.35	0.54
1:G:127:PHE:HD1	1:H:335:LEU:CD2	2.18	0.54
1:E:318:LEU:HG	1:E:318:LEU:O	2.06	0.54
1:B:250:MET:CE	1:B:267:HIS:CE1	2.91	0.53
1:D:250:MET:CE	1:D:267:HIS:CE1	2.91	0.53
1:C:250:MET:CE	1:C:267:HIS:CE1	2.91	0.53
1:H:250:MET:CE	1:H:267:HIS:CE1	2.91	0.53
2:O:104:PHE:HZ	1:G:184:ASN:HD21	1.55	0.53
1:G:109:GLU:OE1	1:H:207:ASN:HB3	2.08	0.53
1:F:250:MET:CE	1:F:267:HIS:CE1	2.91	0.53
1:G:177:LYS:HB2	1:H:62:SER:O	2.08	0.53
1:A:335:LEU:HD21	1:B:127:PHE:CD1	2.44	0.53
1:C:123:ASN:ND2	1:D:204:GLU:OE2	2.42	0.53
1:E:303:ARG:NH2	1:F:130:ILE:O	2.42	0.53
1:C:250:MET:HE2	1:C:267:HIS:CE1	2.44	0.53
1:E:131:ARG:O	1:F:472:MET:HG3	2.10	0.52
1:E:250:MET:HE2	1:E:267:HIS:CD2	2.43	0.52
1:G:250:MET:CE	1:G:267:HIS:CE1	2.91	0.52
1:A:250:MET:CE	1:A:267:HIS:CE1	2.91	0.52
1:B:184:ASN:HD21	2:J:104:PHE:HZ	1.56	0.51
1:F:250:MET:HE2	1:F:267:HIS:CE1	2.45	0.51
1:G:335:LEU:HD21	1:H:127:PHE:CE1	2.45	0.51
1:E:319:ARG:NH2	1:E:351:GLU:O	2.35	0.51
1:E:295:ARG:HD2	1:E:327:HIS:HB2	1.93	0.51
1:A:213:ARG:HD2	4:A:491:HOH:O	2.10	0.51
1:H:31:PRO:HB3	1:H:37:LEU:HD21	1.93	0.51
1:E:335:LEU:HD21	1:F:127:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:104:PHE:HZ	1:E:184:ASN:HD21	1.56	0.51
1:A:31:PRO:HB3	1:A:37:LEU:HD21	1.93	0.51
1:G:66:TRP:CH2	1:H:383:HIS:CD2	2.99	0.51
1:E:335:LEU:CD2	1:F:127:PHE:HD1	2.23	0.51
1:G:31:PRO:HB3	1:G:37:LEU:HD21	1.93	0.51
1:F:31:PRO:HB3	1:F:37:LEU:HD21	1.93	0.51
1:D:31:PRO:HB3	1:D:37:LEU:HD21	1.93	0.51
1:D:295:ARG:HD2	1:D:327:HIS:HB2	1.93	0.51
1:G:246:THR:HG22	1:H:278:THR:HG22	1.93	0.51
1:C:31:PRO:HB3	1:C:37:LEU:HD21	1.93	0.51
1:E:448:ALA:HA	1:E:451:TRP:NE1	2.26	0.51
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.94	0.51
1:C:448:ALA:HA	1:C:451:TRP:NE1	2.26	0.50
1:G:121:VAL:O	1:H:297:MET:HA	2.12	0.50
1:B:295:ARG:HD2	1:B:327:HIS:HB2	1.93	0.50
1:C:295:ARG:HD2	1:C:327:HIS:HB2	1.93	0.50
1:A:295:ARG:HD2	1:A:327:HIS:HB2	1.93	0.50
1:F:250:MET:CE	1:F:267:HIS:HE2	2.23	0.50
1:D:250:MET:CE	1:D:267:HIS:HE2	2.24	0.50
1:E:31:PRO:HB3	1:E:37:LEU:HD21	1.93	0.50
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.94	0.50
1:B:31:PRO:HB3	1:B:37:LEU:HD21	1.93	0.50
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.94	0.50
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.94	0.50
1:A:303:ARG:NH2	1:B:130:ILE:O	2.44	0.50
1:F:448:ALA:HA	1:F:451:TRP:NE1	2.26	0.50
1:B:448:ALA:HA	1:B:451:TRP:NE1	2.26	0.50
1:G:448:ALA:HA	1:G:451:TRP:NE1	2.27	0.50
1:F:295:ARG:HD2	1:F:327:HIS:HB2	1.93	0.50
1:A:153:HIS:HE1	4:A:526:HOH:O	1.94	0.50
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.94	0.50
1:H:295:ARG:HD2	1:H:327:HIS:HB2	1.93	0.50
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.94	0.50
1:H:448:ALA:HA	1:H:451:TRP:NE1	2.26	0.50
1:E:461:LEU:HD21	1:F:15:ALA:HB1	1.93	0.50
1:D:448:ALA:HA	1:D:451:TRP:NE1	2.27	0.50
1:C:381:GLY:HA2	1:D:66:TRP:CD1	2.47	0.50
1:B:250:MET:HE2	1:B:267:HIS:CD2	2.46	0.50
1:G:250:MET:HE2	1:G:267:HIS:CD2	2.47	0.50
1:F:184:ASN:HD21	2:L:104:PHE:HZ	1.57	0.50
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.94	0.50
1:A:448:ALA:HA	1:A:451:TRP:NE1	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:127:PHE:HD1	1:F:335:LEU:HD21	1.76	0.49
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.94	0.49
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.94	0.49
2:O:69:MET:HE3	2:O:71:LYS:O	2.13	0.49
1:A:127:PHE:CD1	1:B:335:LEU:HD23	2.47	0.49
1:G:109:GLU:OE2	1:H:253:ARG:NH2	2.36	0.49
1:E:105:LEU:HD21	1:H:146:LYS:HD2	1.94	0.49
1:A:435:ARG:NH2	1:A:447:GLU:OE1	2.45	0.49
1:G:295:ARG:HD2	1:G:327:HIS:HB2	1.93	0.49
1:F:435:ARG:NH2	1:F:447:GLU:OE1	2.45	0.49
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.94	0.49
1:C:435:ARG:NH2	1:C:447:GLU:OE1	2.45	0.49
1:E:109:GLU:OE2	1:F:253:ARG:NH2	2.28	0.49
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.95	0.49
1:H:435:ARG:NH2	1:H:447:GLU:OE1	2.45	0.49
1:D:435:ARG:NH2	1:D:447:GLU:OE1	2.45	0.49
1:B:250:MET:CE	1:B:267:HIS:HE2	2.23	0.49
1:A:335:LEU:CD2	1:B:127:PHE:HD1	2.25	0.49
1:E:435:ARG:NH2	1:E:447:GLU:OE1	2.46	0.49
1:C:117:LEU:O	1:C:121:VAL:HG22	2.13	0.49
1:F:117:LEU:O	1:F:121:VAL:HG22	2.13	0.49
1:D:250:MET:HE1	1:D:267:HIS:CE1	2.47	0.49
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.94	0.49
1:E:40:PHE:O	1:E:98:PHE:HA	2.13	0.49
1:G:63:THR:HA	1:H:177:LYS:HB2	1.94	0.49
1:B:117:LEU:O	1:B:121:VAL:HG22	2.13	0.49
1:E:117:LEU:O	1:E:121:VAL:HG22	2.13	0.49
1:G:435:ARG:NH2	1:G:447:GLU:OE1	2.45	0.49
1:A:67:THR:CG2	1:B:462:TRP:HE1	2.02	0.49
1:H:250:MET:CE	1:H:267:HIS:HE2	2.23	0.49
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.96	0.49
1:E:177:LYS:HB2	1:F:62:SER:O	2.13	0.49
1:B:435:ARG:NH2	1:B:447:GLU:OE1	2.45	0.49
1:C:204:GLU:OE2	1:D:123:ASN:ND2	2.46	0.49
1:A:40:PHE:O	1:A:98:PHE:HA	2.13	0.49
1:C:65:THR:OG1	3:D:476:XBP:O2P	2.21	0.49
1:H:40:PHE:O	1:H:98:PHE:HA	2.13	0.49
1:G:125:PHE:O	1:H:303:ARG:HD3	2.13	0.48
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.96	0.48
1:A:117:LEU:O	1:A:121:VAL:HG22	2.13	0.48
1:D:40:PHE:O	1:D:98:PHE:HA	2.13	0.48
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:127:PHE:CD1	1:D:335:LEU:HD21	2.48	0.48
1:G:117:LEU:O	1:G:121:VAL:HG22	2.13	0.48
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.96	0.48
1:A:461:LEU:HD21	1:B:15:ALA:HB1	1.93	0.48
1:G:178:LEU:HD12	1:H:107:LEU:HD22	1.94	0.48
1:B:319:ARG:HG2	1:B:368:TRP:CZ3	2.49	0.48
1:C:40:PHE:O	1:C:98:PHE:HA	2.13	0.48
1:F:40:PHE:O	1:F:98:PHE:HA	2.13	0.48
2:J:69:MET:HE3	2:J:71:LYS:O	2.13	0.48
1:D:319:ARG:HG2	1:D:368:TRP:CZ3	2.49	0.48
1:D:414:ALA:HB3	1:D:415:PRO:HD3	1.95	0.48
1:G:205:ASN:HB2	1:H:119:SER:OG	2.14	0.48
1:H:250:MET:HE2	1:H:267:HIS:CD2	2.48	0.48
1:F:229:GLN:HE21	1:F:236:LYS:H	1.62	0.48
1:H:117:LEU:O	1:H:121:VAL:HG22	2.13	0.48
1:A:319:ARG:HG2	1:A:368:TRP:CZ3	2.49	0.48
1:G:318:LEU:HD22	1:G:326:LEU:HD13	1.96	0.48
1:E:319:ARG:HG2	1:E:368:TRP:CZ3	2.49	0.48
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.96	0.48
1:B:40:PHE:O	1:B:98:PHE:HA	2.13	0.48
1:D:295:ARG:HG3	1:D:298:HIS:CD2	2.49	0.48
1:H:319:ARG:NH2	1:H:351:GLU:O	2.35	0.48
1:E:295:ARG:HG3	1:E:298:HIS:CD2	2.49	0.48
1:C:295:ARG:HG3	1:C:298:HIS:CD2	2.49	0.48
2:N:69:MET:HE3	2:N:71:LYS:O	2.14	0.48
1:D:117:LEU:O	1:D:121:VAL:HG22	2.13	0.48
1:E:250:MET:HE1	1:E:267:HIS:CE1	2.49	0.48
1:G:250:MET:CE	1:G:267:HIS:HE2	2.24	0.48
2:P:69:MET:HE3	2:P:72:LEU:HD23	1.95	0.48
1:F:319:ARG:HG2	1:F:368:TRP:CZ3	2.49	0.48
1:F:414:ALA:HB3	1:F:415:PRO:HD3	1.95	0.48
1:G:40:PHE:O	1:G:98:PHE:HA	2.13	0.48
1:E:134:ARG:HA	1:E:308:GLY:O	2.14	0.48
1:B:295:ARG:HG3	1:B:298:HIS:CD2	2.49	0.48
2:L:69:MET:HE3	2:L:71:LYS:O	2.14	0.48
2:I:69:MET:HE3	2:I:71:LYS:O	2.14	0.48
1:C:319:ARG:HG2	1:C:368:TRP:CZ3	2.49	0.48
1:A:472:MET:HG3	1:B:131:ARG:O	2.14	0.48
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.95	0.48
1:H:295:ARG:HG3	1:H:298:HIS:CD2	2.49	0.47
1:G:295:ARG:HG3	1:G:298:HIS:CD2	2.49	0.47
1:A:247:CYS:H	1:B:279:THR:HG1	1.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:318:LEU:HD22	1:C:326:LEU:HD13	1.96	0.47
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.96	0.47
1:G:204:GLU:OE2	1:H:123:ASN:ND2	2.47	0.47
1:C:109:GLU:OE2	1:D:253:ARG:NH2	2.32	0.47
1:B:134:ARG:HA	1:B:308:GLY:O	2.14	0.47
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.49	0.47
1:C:250:MET:CE	1:C:267:HIS:HE2	2.23	0.47
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.96	0.47
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.96	0.47
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.96	0.47
1:H:319:ARG:HG2	1:H:368:TRP:CZ3	2.49	0.47
1:A:146:LYS:HD2	1:D:105:LEU:HD21	1.96	0.47
1:E:49:PRO:HG2	1:E:52:GLU:HB3	1.96	0.47
1:D:134:ARG:HA	1:D:308:GLY:O	2.14	0.47
1:C:49:PRO:HG2	1:C:52:GLU:HB3	1.96	0.47
1:A:177:LYS:HB2	1:B:62:SER:O	2.14	0.47
1:B:49:PRO:HG2	1:B:52:GLU:HB3	1.96	0.47
3:C:476:XPB:O2P	1:D:65:THR:OG1	2.22	0.47
1:A:250:MET:CE	1:A:267:HIS:HE2	2.23	0.47
1:H:250:MET:HE2	1:H:267:HIS:CE1	2.50	0.47
1:D:19:ASP:HB2	1:D:22:LEU:HG	1.97	0.47
2:N:119:ARG:HG3	2:N:119:ARG:HH11	1.79	0.47
1:G:134:ARG:HA	1:G:308:GLY:O	2.15	0.47
1:F:295:ARG:HG3	1:F:298:HIS:CD2	2.49	0.47
2:M:69:MET:HE3	2:M:71:LYS:O	2.14	0.47
1:C:335:LEU:HD21	1:D:127:PHE:CD1	2.50	0.47
1:A:318:LEU:HD22	1:A:326:LEU:HD13	1.96	0.47
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.49	0.47
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.49	0.47
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.49	0.47
2:K:119:ARG:HH11	2:K:119:ARG:HG3	1.79	0.47
2:M:119:ARG:HG3	2:M:119:ARG:HH11	1.79	0.47
1:B:318:LEU:HD22	1:B:326:LEU:HD13	1.96	0.47
1:F:166:GLY:HA2	2:K:112:THR:O	2.15	0.47
1:H:19:ASP:HB2	1:H:22:LEU:HG	1.96	0.47
1:E:119:SER:OG	1:F:205:ASN:HB2	2.14	0.47
1:F:134:ARG:HA	1:F:308:GLY:O	2.14	0.47
1:H:49:PRO:HG2	1:H:52:GLU:HB3	1.96	0.47
1:G:166:GLY:HA2	2:P:112:THR:O	2.15	0.47
1:A:19:ASP:HB2	1:A:22:LEU:HG	1.96	0.47
1:C:250:MET:HE1	1:C:276:ALA:HB1	1.96	0.47
1:D:229:GLN:HE21	1:D:236:LYS:H	1.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:229:GLN:HE21	1:H:236:LYS:H	1.62	0.47
1:F:318:LEU:HD22	1:F:326:LEU:HD13	1.96	0.47
1:E:318:LEU:HD22	1:E:326:LEU:HD13	1.96	0.47
1:A:447:GLU:O	1:A:450:LYS:HB2	2.15	0.47
1:D:447:GLU:O	1:D:450:LYS:HB2	2.15	0.47
1:C:134:ARG:HA	1:C:308:GLY:O	2.14	0.47
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.49	0.47
2:L:119:ARG:HH11	2:L:119:ARG:HG3	1.79	0.47
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.49	0.47
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.49	0.47
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.50	0.47
1:H:166:GLY:HA2	2:L:112:THR:O	2.15	0.47
1:A:49:PRO:HG2	1:A:52:GLU:HB3	1.96	0.47
2:I:119:ARG:HH11	2:I:119:ARG:HG3	1.79	0.47
1:G:319:ARG:HG2	1:G:368:TRP:CZ3	2.49	0.47
1:B:229:GLN:HE21	1:B:236:LYS:H	1.62	0.47
1:C:229:GLN:HE21	1:C:236:LYS:H	1.62	0.47
1:F:447:GLU:O	1:F:450:LYS:HB2	2.15	0.47
1:B:166:GLY:HA2	2:I:112:THR:O	2.15	0.47
1:C:19:ASP:HB2	1:C:22:LEU:HG	1.96	0.47
1:G:65:THR:OG1	3:H:476:XBP:O2P	2.14	0.47
2:K:69:MET:HE3	2:K:71:LYS:O	2.14	0.47
1:G:229:GLN:HE21	1:G:236:LYS:H	1.62	0.47
1:G:185:TYR:OH	1:G:202:ASP:HA	2.15	0.47
1:G:49:PRO:HG2	1:G:52:GLU:HB3	1.96	0.47
1:E:447:GLU:O	1:E:450:LYS:HB2	2.15	0.47
1:B:447:GLU:O	1:B:450:LYS:HB2	2.15	0.47
1:G:19:ASP:HB2	1:G:22:LEU:HG	1.96	0.47
1:E:159:ARG:NH2	1:E:167:ARG:O	2.46	0.47
1:E:19:ASP:HB2	1:E:22:LEU:HG	1.97	0.47
1:A:130:ILE:O	1:B:303:ARG:NH2	2.44	0.47
1:A:134:ARG:HA	1:A:308:GLY:O	2.14	0.46
1:H:159:ARG:NH2	1:H:167:ARG:O	2.47	0.46
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.49	0.46
2:O:119:ARG:HH11	2:O:119:ARG:HG3	1.79	0.46
1:F:152:PRO:HB2	1:F:153:HIS:CD2	2.49	0.46
1:H:134:ARG:HA	1:H:308:GLY:O	2.14	0.46
1:A:127:PHE:HD1	1:B:335:LEU:CD2	2.28	0.46
1:G:447:GLU:O	1:G:450:LYS:HB2	2.15	0.46
1:B:19:ASP:HB2	1:B:22:LEU:HG	1.97	0.46
1:E:207:ASN:HB3	1:F:109:GLU:OE1	2.15	0.46
1:C:166:GLY:HA2	2:N:112:THR:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:119:ARG:HH11	2:P:119:ARG:HG3	1.80	0.46
1:E:166:GLY:HA2	2:O:112:THR:O	2.15	0.46
1:E:229:GLN:HE21	1:E:236:LYS:H	1.62	0.46
1:E:185:TYR:OH	1:E:202:ASP:HA	2.16	0.46
1:A:166:GLY:HA2	2:M:112:THR:O	2.15	0.46
2:J:119:ARG:HG3	2:J:119:ARG:HH11	1.79	0.46
1:D:318:LEU:HD22	1:D:326:LEU:HD13	1.96	0.46
1:H:447:GLU:O	1:H:450:LYS:HB2	2.15	0.46
1:F:19:ASP:HB2	1:F:22:LEU:HG	1.96	0.46
1:H:318:LEU:HD22	1:H:326:LEU:HD13	1.96	0.46
1:D:185:TYR:OH	1:D:202:ASP:HA	2.16	0.46
1:F:49:PRO:HG2	1:F:52:GLU:HB3	1.96	0.46
1:A:229:GLN:HE21	1:A:236:LYS:H	1.62	0.46
1:C:185:TYR:OH	1:C:202:ASP:HA	2.16	0.46
1:F:185:TYR:OH	1:F:202:ASP:HA	2.16	0.46
1:F:250:MET:HE1	1:F:276:ALA:HB1	1.97	0.46
1:C:335:LEU:HD23	1:D:127:PHE:CD1	2.50	0.46
1:H:185:TYR:OH	1:H:202:ASP:HA	2.16	0.46
1:A:185:TYR:OH	1:A:202:ASP:HA	2.16	0.46
1:D:49:PRO:HG2	1:D:52:GLU:HB3	1.96	0.46
1:B:185:TYR:OH	1:B:202:ASP:HA	2.16	0.45
1:G:383:HIS:HD2	1:H:66:TRP:CH2	2.34	0.45
1:C:447:GLU:O	1:C:450:LYS:HB2	2.15	0.45
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.51	0.45
1:D:166:GLY:HA2	2:J:112:THR:O	2.15	0.45
1:G:62:SER:O	1:H:177:LYS:HB2	2.16	0.45
1:E:45:GLN:NE2	1:F:470:GLU:O	2.48	0.45
1:C:461:LEU:HD21	1:D:15:ALA:HB1	1.99	0.45
1:F:295:ARG:HG3	1:F:298:HIS:CG	2.52	0.45
1:E:295:ARG:HG3	1:E:298:HIS:CG	2.52	0.45
1:A:295:ARG:HG3	1:A:298:HIS:CG	2.52	0.45
1:G:178:LEU:HD13	1:H:107:LEU:HD22	1.98	0.45
1:E:383:HIS:HD2	1:F:66:TRP:CH2	2.35	0.45
1:A:204:GLU:OE2	1:B:123:ASN:ND2	2.50	0.45
1:D:295:ARG:HG3	1:D:298:HIS:CG	2.52	0.45
1:B:295:ARG:HG3	1:B:298:HIS:CG	2.52	0.45
1:D:293:ILE:HG21	1:D:318:LEU:HD13	1.99	0.45
1:F:250:MET:HE2	1:F:267:HIS:CD2	2.51	0.45
1:H:293:ILE:HG21	1:H:318:LEU:HD13	1.99	0.45
1:C:295:ARG:HG3	1:C:298:HIS:CG	2.52	0.44
1:G:295:ARG:HG3	1:G:298:HIS:CG	2.52	0.44
1:B:293:ILE:HG21	1:B:318:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:293:ILE:HG21	1:G:318:LEU:HD13	1.99	0.44
1:H:295:ARG:HG3	1:H:298:HIS:CG	2.52	0.44
1:E:250:MET:CE	1:E:267:HIS:HE2	2.23	0.44
1:A:293:ILE:HG21	1:A:318:LEU:HD13	1.99	0.44
1:F:293:ILE:HG21	1:F:318:LEU:HD13	1.99	0.44
1:E:293:ILE:HG21	1:E:318:LEU:HD13	2.00	0.44
1:A:105:LEU:HD21	1:D:146:LYS:HD2	1.99	0.44
1:A:250:MET:HE3	1:A:276:ALA:HB1	2.00	0.44
1:G:66:TRP:CG	1:H:381:GLY:HA2	2.52	0.44
1:C:127:PHE:CD1	1:D:335:LEU:HD23	2.52	0.44
1:C:293:ILE:HG21	1:C:318:LEU:HD13	1.99	0.44
1:G:250:MET:HE2	1:G:267:HIS:CE1	2.52	0.44
1:G:381:GLY:HA2	1:H:66:TRP:CG	2.52	0.44
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.66	0.44
1:H:383:HIS:CE1	1:H:385:TRP:HB2	2.53	0.44
1:A:130:ILE:HD13	1:A:130:ILE:HA	1.86	0.44
1:C:253:ARG:NH2	1:D:109:GLU:OE2	2.35	0.44
1:H:130:ILE:HD13	1:H:130:ILE:HA	1.86	0.44
1:G:207:ASN:HB3	1:H:109:GLU:OE1	2.18	0.44
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.53	0.44
1:C:152:PRO:O	1:C:285:ARG:HD3	2.18	0.44
1:A:159:ARG:NH2	1:A:167:ARG:O	2.47	0.44
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.66	0.44
2:O:14:THR:O	2:O:15:PHE:HB2	2.18	0.44
1:D:383:HIS:CE1	1:D:385:TRP:HB2	2.53	0.44
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.53	0.44
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.53	0.44
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.53	0.44
1:D:152:PRO:O	1:D:285:ARG:HD3	2.18	0.44
1:G:152:PRO:O	1:G:285:ARG:HD3	2.18	0.44
1:A:195:GLY:HA3	1:A:417:ALA:HB3	2.00	0.44
1:F:195:GLY:HA3	1:F:417:ALA:HB3	2.00	0.44
1:F:152:PRO:O	1:F:285:ARG:HD3	2.18	0.43
1:B:159:ARG:NH2	1:B:167:ARG:O	2.47	0.43
1:E:178:LEU:CD1	1:F:107:LEU:HD22	2.48	0.43
1:A:131:ARG:O	1:B:472:MET:HG3	2.18	0.43
1:C:293:ILE:HG21	1:C:318:LEU:CD1	2.49	0.43
1:B:152:PRO:O	1:B:285:ARG:HD3	2.18	0.43
1:E:470:GLU:O	1:F:45:GLN:NE2	2.50	0.43
1:C:130:ILE:HD13	1:C:130:ILE:HA	1.86	0.43
1:D:159:ARG:NH2	1:D:167:ARG:O	2.47	0.43
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293:ILE:HG21	1:B:318:LEU:CD1	2.49	0.43
1:A:293:ILE:HG21	1:A:318:LEU:CD1	2.49	0.43
1:G:293:ILE:HG21	1:G:318:LEU:CD1	2.48	0.43
2:P:33:MET:HE1	2:P:101:VAL:HG12	1.99	0.43
1:A:62:SER:O	1:B:177:LYS:HB2	2.18	0.43
1:E:63:THR:HA	1:F:177:LYS:HB2	1.99	0.43
2:M:14:THR:O	2:M:15:PHE:HB2	2.19	0.43
2:N:14:THR:O	2:N:15:PHE:HB2	2.19	0.43
1:D:195:GLY:HA3	1:D:417:ALA:HB3	2.00	0.43
2:O:11:ARG:HG3	2:O:17:TYR:CE1	2.54	0.43
2:P:14:THR:O	2:P:15:PHE:HB2	2.19	0.43
2:J:14:THR:O	2:J:15:PHE:HB2	2.19	0.43
1:G:114:THR:HG23	1:H:271:THR:C	2.39	0.43
1:H:152:PRO:O	1:H:285:ARG:HD3	2.18	0.43
1:C:239:TYR:HB3	1:C:266:MET:HB2	2.01	0.43
2:L:14:THR:O	2:L:15:PHE:HB2	2.19	0.43
2:K:14:THR:O	2:K:15:PHE:HB2	2.19	0.43
2:J:11:ARG:HG3	2:J:17:TYR:CE1	2.54	0.43
2:O:6:LEU:HA	2:O:7:PRO:HD3	1.92	0.43
1:E:279:THR:HG1	1:F:247:CYS:H	1.67	0.43
1:C:195:GLY:HA3	1:C:417:ALA:HB3	2.00	0.43
1:B:239:TYR:HB3	1:B:266:MET:HB2	2.01	0.43
2:I:19:PRO:HA	2:I:20:PRO:HD3	1.90	0.43
1:E:195:GLY:HA3	1:E:417:ALA:HB3	2.00	0.43
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.54	0.43
1:E:128:LYS:HD2	1:F:333:GLY:O	2.18	0.43
1:D:293:ILE:HG21	1:D:318:LEU:CD1	2.49	0.43
1:E:239:TYR:HB3	1:E:266:MET:HB2	2.01	0.43
2:M:19:PRO:HA	2:M:20:PRO:HD3	1.90	0.43
2:N:11:ARG:HG3	2:N:17:TYR:CE1	2.54	0.43
2:I:11:ARG:HG3	2:I:17:TYR:CE1	2.54	0.43
2:P:19:PRO:HA	2:P:20:PRO:HD3	1.91	0.43
1:G:195:GLY:HA3	1:G:417:ALA:HB3	2.00	0.43
1:E:383:HIS:CE1	1:E:385:TRP:HB2	2.54	0.43
1:F:293:ILE:HG21	1:F:318:LEU:CD1	2.49	0.43
1:A:152:PRO:O	1:A:285:ARG:HD3	2.18	0.43
1:A:207:ASN:HB3	1:B:109:GLU:OE1	2.18	0.43
1:E:152:PRO:O	1:E:285:ARG:HD3	2.18	0.43
2:J:33:MET:HE1	2:J:101:VAL:HG12	2.01	0.43
1:B:195:GLY:HA3	1:B:417:ALA:HB3	2.00	0.43
1:H:293:ILE:HG21	1:H:318:LEU:CD1	2.49	0.42
1:D:204:GLU:OE1	1:D:294:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.66	0.42
2:I:14:THR:O	2:I:15:PHE:HB2	2.19	0.42
1:D:171:GLY:HA2	1:D:199:PHE:O	2.19	0.42
1:A:383:HIS:HD2	1:B:66:TRP:CH2	2.37	0.42
1:B:204:GLU:OE1	1:B:294:HIS:CE1	2.72	0.42
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.66	0.42
2:L:11:ARG:HG3	2:L:17:TYR:CE1	2.54	0.42
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.55	0.42
1:E:107:LEU:HD22	1:F:178:LEU:CD1	2.50	0.42
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.66	0.42
1:E:171:GLY:HA2	1:E:199:PHE:O	2.19	0.42
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.66	0.42
1:F:204:GLU:OE1	1:F:294:HIS:CE1	2.72	0.42
1:E:293:ILE:HG21	1:E:318:LEU:CD1	2.49	0.42
1:H:195:GLY:HA3	1:H:417:ALA:HB3	2.00	0.42
2:M:11:ARG:HG3	2:M:17:TYR:CE1	2.54	0.42
1:A:171:GLY:HA2	1:A:199:PHE:O	2.19	0.42
1:E:190:TYR:CZ	1:E:227:LYS:HE3	2.54	0.42
2:P:11:ARG:HG3	2:P:17:TYR:CE1	2.54	0.42
2:O:33:MET:HE1	2:O:101:VAL:HG12	2.01	0.42
1:H:204:GLU:OE1	1:H:294:HIS:CE1	2.72	0.42
2:O:95:GLY:O	2:O:118:HIS:HE1	2.03	0.42
1:C:177:LYS:HB2	1:D:62:SER:O	2.20	0.42
1:A:24:TYR:CE1	1:A:81:LYS:HB2	2.55	0.42
1:D:24:TYR:CE1	1:D:81:LYS:HB2	2.55	0.42
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.55	0.42
1:B:24:TYR:CE1	1:B:81:LYS:HB2	2.55	0.42
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.55	0.42
1:B:133:LEU:O	1:B:307:HIS:HA	2.20	0.42
1:C:250:MET:HE2	1:C:267:HIS:CD2	2.53	0.42
1:G:204:GLU:OE1	1:G:294:HIS:CE1	2.72	0.42
1:H:239:TYR:HB3	1:H:266:MET:HB2	2.01	0.42
1:B:136:GLU:OE1	1:B:312:ARG:NH2	2.53	0.42
1:C:136:GLU:OE1	1:C:312:ARG:NH2	2.53	0.42
1:D:136:GLU:OE1	1:D:312:ARG:NH2	2.53	0.42
1:H:24:TYR:CE1	1:H:81:LYS:HB2	2.55	0.42
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.55	0.42
2:I:95:GLY:O	2:I:118:HIS:HE1	2.03	0.42
1:G:71:THR:HG21	1:H:407:LEU:HD23	2.00	0.42
1:C:133:LEU:O	1:C:307:HIS:HA	2.20	0.42
1:E:204:GLU:OE1	1:E:294:HIS:CE1	2.73	0.42
1:G:171:GLY:HA2	1:G:199:PHE:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:11:ARG:HG3	2:K:17:TYR:CE1	2.54	0.42
2:N:95:GLY:O	2:N:118:HIS:HE1	2.03	0.42
1:E:136:GLU:OE1	1:E:312:ARG:NH2	2.53	0.42
1:G:136:GLU:OE1	1:G:312:ARG:NH2	2.53	0.42
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.66	0.42
1:A:136:GLU:OE1	1:A:312:ARG:NH2	2.53	0.42
1:H:250:MET:HE1	1:H:276:ALA:HB1	2.02	0.42
2:P:69:MET:HE3	2:P:71:LYS:O	2.19	0.42
1:E:130:ILE:HA	1:E:130:ILE:HD13	1.87	0.42
1:C:204:GLU:OE1	1:C:294:HIS:CE1	2.72	0.42
1:A:470:GLU:O	1:B:45:GLN:NE2	2.53	0.42
1:G:24:TYR:CE1	1:G:81:LYS:HB2	2.55	0.42
1:B:250:MET:HE1	1:B:267:HIS:CE1	2.55	0.42
1:E:410:PRO:HD3	1:E:461:LEU:HD22	2.02	0.42
1:A:204:GLU:OE1	1:A:294:HIS:CE1	2.72	0.42
2:L:19:PRO:HA	2:L:20:PRO:HD3	1.90	0.42
1:C:24:TYR:CE1	1:C:81:LYS:HB2	2.55	0.42
1:F:171:GLY:HA2	1:F:199:PHE:O	2.20	0.42
1:D:239:TYR:HB3	1:D:266:MET:HB2	2.01	0.42
1:F:24:TYR:CE1	1:F:81:LYS:HB2	2.55	0.42
1:E:178:LEU:HD12	1:F:107:LEU:HD22	2.01	0.42
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.02	0.42
1:H:136:GLU:OE1	1:H:312:ARG:NH2	2.53	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.20	0.42
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.55	0.42
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.42
1:E:133:LEU:O	1:E:307:HIS:HA	2.20	0.42
1:F:136:GLU:OE1	1:F:312:ARG:NH2	2.53	0.42
2:M:104:PHE:HZ	1:C:184:ASN:HD21	1.64	0.42
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.55	0.42
1:C:247:CYS:H	1:D:279:THR:HG1	1.67	0.42
1:F:197:LEU:HG	1:F:417:ALA:HB1	2.02	0.42
1:F:239:TYR:HB3	1:F:266:MET:HB2	2.01	0.42
2:P:6:LEU:HA	2:P:7:PRO:HD3	1.92	0.42
2:J:6:LEU:HA	2:J:7:PRO:HD3	1.92	0.42
1:B:353:HIS:HD2	1:B:367:ASP:OD1	2.03	0.42
1:G:461:LEU:CD2	1:H:15:ALA:HB1	2.49	0.41
1:A:239:TYR:HB3	1:A:266:MET:HB2	2.01	0.41
2:J:95:GLY:O	2:J:118:HIS:HE1	2.03	0.41
1:E:146:LYS:HD2	1:H:105:LEU:HD21	2.03	0.41
1:A:133:LEU:O	1:A:307:HIS:HA	2.20	0.41
1:G:239:TYR:HB3	1:G:266:MET:HB2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.66	0.41
1:F:159:ARG:NH2	1:F:167:ARG:O	2.47	0.41
1:E:353:HIS:HD2	1:E:367:ASP:OD1	2.03	0.41
2:K:95:GLY:O	2:K:118:HIS:HE1	2.03	0.41
2:M:45:ASN:HB2	2:M:67:TRP:CD2	2.55	0.41
2:L:95:GLY:O	2:L:118:HIS:HE1	2.03	0.41
1:F:133:LEU:O	1:F:307:HIS:HA	2.20	0.41
2:I:13:GLU:HB3	2:I:14:THR:H	1.73	0.41
2:J:45:ASN:HB2	2:J:67:TRP:CD2	2.56	0.41
1:H:171:GLY:HA2	1:H:199:PHE:O	2.19	0.41
1:H:353:HIS:HD2	1:H:367:ASP:OD1	2.03	0.41
1:C:353:HIS:HD2	1:C:367:ASP:OD1	2.03	0.41
1:A:226:HIS:HE1	4:A:487:HOH:O	2.03	0.41
1:C:62:SER:O	1:D:177:LYS:HB2	2.21	0.41
1:A:410:PRO:HD3	1:A:461:LEU:HD22	2.02	0.41
1:E:278:THR:HG22	1:F:246:THR:HG22	2.02	0.41
1:F:190:TYR:CZ	1:F:227:LYS:HE3	2.55	0.41
1:D:133:LEU:O	1:D:307:HIS:HA	2.20	0.41
2:O:10:ARG:O	2:O:11:ARG:HD2	2.21	0.41
1:B:410:PRO:HD3	1:B:461:LEU:HD22	2.02	0.41
1:C:171:GLY:HA2	1:C:199:PHE:O	2.19	0.41
2:M:95:GLY:O	2:M:118:HIS:HE1	2.03	0.41
1:G:133:LEU:O	1:G:307:HIS:HA	2.20	0.41
1:D:410:PRO:HD3	1:D:461:LEU:HD22	2.02	0.41
1:H:410:PRO:HD3	1:H:461:LEU:HD22	2.02	0.41
1:G:127:PHE:CE1	1:H:335:LEU:HD21	2.56	0.41
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.03	0.41
2:M:118:HIS:HD2	4:M:155:HOH:O	2.02	0.41
2:I:45:ASN:HB2	2:I:67:TRP:CD2	2.56	0.41
1:F:353:HIS:HD2	1:F:367:ASP:OD1	2.03	0.41
1:G:159:ARG:NH2	1:G:167:ARG:O	2.47	0.41
2:L:45:ASN:HB2	2:L:67:TRP:CD2	2.55	0.41
2:M:33:MET:HE1	2:M:101:VAL:HG12	2.03	0.41
1:C:410:PRO:HD3	1:C:461:LEU:HD22	2.02	0.41
2:K:45:ASN:HB2	2:K:67:TRP:CD2	2.56	0.41
1:E:24:TYR:CE1	1:E:81:LYS:HB2	2.55	0.41
1:F:130:ILE:HD13	1:F:130:ILE:HA	1.86	0.41
1:G:247:CYS:H	1:H:279:THR:HG1	1.69	0.41
1:D:197:LEU:HG	1:D:417:ALA:HB1	2.02	0.41
2:P:95:GLY:O	2:P:118:HIS:HE1	2.03	0.41
1:E:15:ALA:HB1	1:F:461:LEU:HD21	2.03	0.41
1:A:353:HIS:HD2	1:A:367:ASP:OD1	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:371:MET:HA	1:C:372:PRO:HD3	1.97	0.41
1:B:250:MET:HE2	1:B:267:HIS:CE1	2.53	0.41
1:G:214:TRP:CD2	1:G:253:ARG:HG2	2.56	0.41
1:C:130:ILE:O	1:D:303:ARG:NH2	2.54	0.41
1:H:197:LEU:HG	1:H:417:ALA:HB1	2.02	0.41
2:I:104:PHE:HZ	1:H:184:ASN:HD21	1.63	0.41
1:C:159:ARG:NH2	1:C:167:ARG:O	2.47	0.41
2:M:6:LEU:HA	2:M:7:PRO:HD3	1.92	0.41
1:E:121:VAL:O	1:F:297:MET:HA	2.21	0.40
1:A:197:LEU:HG	1:A:417:ALA:HB1	2.02	0.40
2:J:10:ARG:O	2:J:11:ARG:HD2	2.21	0.40
2:L:10:ARG:O	2:L:11:ARG:HD2	2.21	0.40
1:G:71:THR:CG2	1:H:407:LEU:HD23	2.51	0.40
1:F:410:PRO:HD3	1:F:461:LEU:HD22	2.02	0.40
1:G:353:HIS:HD2	1:G:367:ASP:OD1	2.04	0.40
2:N:45:ASN:HB2	2:N:67:TRP:CD2	2.55	0.40
2:N:6:LEU:HA	2:N:7:PRO:HD3	1.92	0.40
1:C:105:LEU:HD21	1:F:146:LYS:HD2	2.03	0.40
1:C:279:THR:HG1	1:D:247:CYS:H	1.69	0.40
2:O:13:GLU:HB3	2:O:14:THR:H	1.73	0.40
2:I:10:ARG:O	2:I:11:ARG:HD2	2.21	0.40
2:P:10:ARG:O	2:P:11:ARG:HD2	2.21	0.40
2:L:6:LEU:HA	2:L:7:PRO:HD3	1.92	0.40
1:C:146:LYS:HD2	1:F:105:LEU:HD21	2.03	0.40
1:B:377:VAL:HG22	1:B:399:VAL:HB	2.03	0.40
2:O:45:ASN:HB2	2:O:67:TRP:CD2	2.55	0.40
2:P:45:ASN:HB2	2:P:67:TRP:CD2	2.56	0.40
2:O:11:ARG:HH21	2:O:17:TYR:HA	1.87	0.40
2:J:11:ARG:HH21	2:J:17:TYR:HA	1.87	0.40
2:N:11:ARG:HH21	2:N:17:TYR:HA	1.87	0.40
2:P:11:ARG:HH21	2:P:17:TYR:HA	1.87	0.40
1:C:377:VAL:HG22	1:C:399:VAL:HB	2.03	0.40
1:D:353:HIS:HD2	1:D:367:ASP:OD1	2.03	0.40
1:E:68:THR:O	1:F:408:GLY:HA2	2.21	0.40
1:H:214:TRP:CD2	1:H:253:ARG:HG2	2.57	0.40
1:E:109:GLU:OE1	1:F:207:ASN:HB3	2.21	0.40
1:C:197:LEU:HG	1:C:417:ALA:HB1	2.02	0.40
2:K:11:ARG:HG3	2:K:17:TYR:CZ	2.57	0.40
1:C:303:ARG:NH2	1:D:130:ILE:O	2.54	0.40
1:E:44:PRO:HA	1:E:130:ILE:HD13	2.03	0.40
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.86	0.40
1:F:214:TRP:CD2	1:F:253:ARG:HG2	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:207:ASN:HB3	1:D:109:GLU:OE1	2.22	0.40
1:C:214:TRP:CD2	1:C:253:ARG:HG2	2.57	0.40
2:M:10:ARG:O	2:M:11:ARG:HD2	2.21	0.40
1:F:377:VAL:HG22	1:F:399:VAL:HB	2.03	0.40
1:A:109:GLU:OE2	1:B:253:ARG:NH2	2.35	0.40
1:B:214:TRP:CD2	1:B:253:ARG:HG2	2.57	0.40

All (32) 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)
2:O:24:ARG:CZ	2:K:21:LEU:C[2_554]	0.17	2.03
2:O:81:GLN:NE2	2:K:24:ARG:NH1[2_554]	0.59	1.61
2:O:81:GLN:CG	2:K:24:ARG:NH2[2_554]	0.80	1.40
2:O:81:GLN:NE2	2:K:24:ARG:CZ[2_554]	1.03	1.17
2:O:24:ARG:NH1	2:K:21:LEU:CA[2_554]	1.05	1.15
2:O:81:GLN:CD	2:K:24:ARG:CZ[2_554]	1.17	1.03
2:O:24:ARG:CZ	2:K:22:SER:N[2_554]	1.20	1.00
2:O:24:ARG:NH2	2:K:21:LEU:C[2_554]	1.20	1.00
2:O:24:ARG:CZ	2:K:21:LEU:O[2_554]	1.33	0.87
2:O:24:ARG:NE	2:K:21:LEU:O[2_554]	1.35	0.85
2:O:24:ARG:NH1	2:K:21:LEU:C[2_554]	1.40	0.80
2:O:24:ARG:NE	2:K:21:LEU:C[2_554]	1.41	0.79
2:O:81:GLN:CD	2:K:24:ARG:NH2[2_554]	1.42	0.78
2:O:24:ARG:NH2	2:K:21:LEU:O[2_554]	1.51	0.69
2:O:24:ARG:CZ	2:K:21:LEU:CA[2_554]	1.56	0.64
2:O:24:ARG:NE	2:K:22:SER:N[2_554]	1.67	0.53
2:O:24:ARG:NH1	2:K:22:SER:N[2_554]	1.73	0.47
2:O:81:GLN:CD	2:K:24:ARG:NH1[2_554]	1.73	0.47
2:O:81:GLN:CG	2:K:24:ARG:CZ[2_554]	1.89	0.31
2:O:81:GLN:NE2	2:K:24:ARG:NE[2_554]	1.89	0.31
2:O:24:ARG:NH2	2:K:22:SER:N[2_554]	1.97	0.23
2:O:24:ARG:NH1	2:K:21:LEU:N[2_554]	1.99	0.21
2:O:24:ARG:NH2	2:K:21:LEU:CA[2_554]	2.03	0.17
2:O:81:GLN:CB	2:K:24:ARG:NH2[2_554]	2.06	0.14
2:O:24:ARG:NH2	2:K:22:SER:O[2_554]	2.07	0.13
2:O:81:GLN:CD	2:K:24:ARG:NE[2_554]	2.09	0.11
2:M:24:ARG:NH1	1:C:433:GLU:O[3_654]	2.11	0.09
2:O:81:GLN:NE2	2:K:24:ARG:NH2[2_554]	2.13	0.07
2:O:24:ARG:NE	2:K:22:SER:CA[2_554]	2.14	0.06
2:I:28:ALA:CB	2:J:24:ARG:CZ[3_655]	2.15	0.05
2:O:24:ARG:NH2	2:K:21:LEU:CB[2_554]	2.18	0.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:81:GLN:OE1	2:K:24:ARG:CZ[2_554]	2.19	0.01

## 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	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	B	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	C	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	D	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	E	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	F	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	G	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
1	H	465/472 (98%)	451 (97%)	14 (3%)	0	100	100
2	I	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	J	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	K	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	L	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	M	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	N	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	O	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
2	P	107/111 (96%)	98 (92%)	9 (8%)	0	100	100
All	All	4576/4664 (98%)	4392 (96%)	184 (4%)	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	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	B	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	C	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	D	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	E	377/383 (98%)	356 (94%)	21 (6%)	30	38
1	F	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	G	377/383 (98%)	357 (95%)	20 (5%)	32	41
1	H	377/383 (98%)	356 (94%)	21 (6%)	30	38
2	I	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	J	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	K	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	L	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	M	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	N	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	O	99/104 (95%)	98 (99%)	1 (1%)	85	94
2	P	99/104 (95%)	98 (99%)	1 (1%)	85	94
All	All	3808/3896 (98%)	3638 (96%)	170 (4%)	38	50

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	67	THR
1	A	79	ARG
1	A	96	SER
1	A	127	PHE
1	A	134	ARG
1	A	170	LEU
1	A	213	ARG
1	A	215	ARG
1	A	239	TYR
1	A	241	ASN
1	A	255	GLU
1	A	258	LYS
1	A	285	ARG

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Mol	Chain	Res	Type
1	A	295	ARG
1	A	360	ARG
1	A	375	LEU
1	A	401	GLN
1	A	468	GLU
1	A	471	THR
2	M	106	ASN
1	B	14	LYS
1	B	67	THR
1	B	79	ARG
1	B	96	SER
1	B	127	PHE
1	B	134	ARG
1	B	170	LEU
1	B	213	ARG
1	B	215	ARG
1	B	239	TYR
1	B	241	ASN
1	B	255	GLU
1	B	258	LYS
1	B	285	ARG
1	B	295	ARG
1	B	360	ARG
1	B	375	LEU
1	B	401	GLN
1	B	468	GLU
1	B	471	THR
2	I	106	ASN
1	C	14	LYS
1	C	67	THR
1	C	79	ARG
1	C	96	SER
1	C	127	PHE
1	C	134	ARG
1	C	170	LEU
1	C	213	ARG
1	C	215	ARG
1	C	239	TYR
1	C	241	ASN
1	C	255	GLU
1	C	258	LYS
1	C	285	ARG

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Mol	Chain	Res	Type
1	C	295	ARG
1	C	360	ARG
1	C	375	LEU
1	C	401	GLN
1	C	468	GLU
1	C	471	THR
2	N	106	ASN
1	D	14	LYS
1	D	67	THR
1	D	79	ARG
1	D	96	SER
1	D	127	PHE
1	D	134	ARG
1	D	170	LEU
1	D	213	ARG
1	D	215	ARG
1	D	239	TYR
1	D	241	ASN
1	D	255	GLU
1	D	258	LYS
1	D	285	ARG
1	D	295	ARG
1	D	360	ARG
1	D	375	LEU
1	D	401	GLN
1	D	468	GLU
1	D	471	THR
2	J	106	ASN
1	E	14	LYS
1	E	67	THR
1	E	79	ARG
1	E	96	SER
1	E	127	PHE
1	E	134	ARG
1	E	170	LEU
1	E	213	ARG
1	E	215	ARG
1	E	239	TYR
1	E	241	ASN
1	E	255	GLU
1	E	258	LYS
1	E	285	ARG

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Mol	Chain	Res	Type
1	E	295	ARG
1	E	319	ARG
1	E	360	ARG
1	E	375	LEU
1	E	401	GLN
1	E	468	GLU
1	E	471	THR
2	O	106	ASN
1	F	14	LYS
1	F	67	THR
1	F	79	ARG
1	F	96	SER
1	F	127	PHE
1	F	134	ARG
1	F	170	LEU
1	F	213	ARG
1	F	215	ARG
1	F	239	TYR
1	F	241	ASN
1	F	255	GLU
1	F	258	LYS
1	F	285	ARG
1	F	295	ARG
1	F	360	ARG
1	F	375	LEU
1	F	401	GLN
1	F	468	GLU
1	F	471	THR
2	K	106	ASN
1	G	14	LYS
1	G	67	THR
1	G	79	ARG
1	G	96	SER
1	G	127	PHE
1	G	134	ARG
1	G	170	LEU
1	G	213	ARG
1	G	215	ARG
1	G	239	TYR
1	G	241	ASN
1	G	255	GLU
1	G	258	LYS

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Mol	Chain	Res	Type
1	G	285	ARG
1	G	295	ARG
1	G	360	ARG
1	G	375	LEU
1	G	401	GLN
1	G	468	GLU
1	G	471	THR
2	P	106	ASN
1	H	14	LYS
1	H	67	THR
1	H	79	ARG
1	H	96	SER
1	H	127	PHE
1	H	134	ARG
1	H	170	LEU
1	H	213	ARG
1	H	215	ARG
1	H	239	TYR
1	H	241	ASN
1	H	255	GLU
1	H	258	LYS
1	H	285	ARG
1	H	295	ARG
1	H	319	ARG
1	H	360	ARG
1	H	375	LEU
1	H	401	GLN
1	H	468	GLU
1	H	471	THR
2	L	106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	156	GLN
1	A	226	HIS
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	277	ASN
1	A	304	GLN

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Mol	Chain	Res	Type
1	A	353	HIS
1	A	386	HIS
1	A	401	GLN
1	A	420	ASN
2	M	106	ASN
2	M	118	HIS
1	B	153	HIS
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	277	ASN
1	B	304	GLN
1	B	353	HIS
1	B	386	HIS
1	B	401	GLN
1	B	420	ASN
2	I	106	ASN
2	I	118	HIS
1	C	153	HIS
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	277	ASN
1	C	304	GLN
1	C	353	HIS
1	C	386	HIS
1	C	401	GLN
1	C	420	ASN
2	N	106	ASN
2	N	118	HIS
1	D	153	HIS
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN
1	D	277	ASN
1	D	304	GLN
1	D	353	HIS
1	D	386	HIS
1	D	401	GLN
1	D	420	ASN
2	J	106	ASN
2	J	118	HIS

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Mol	Chain	Res	Type
1	E	153	HIS
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	277	ASN
1	E	304	GLN
1	E	353	HIS
1	E	383	HIS
1	E	386	HIS
1	E	401	GLN
1	E	420	ASN
2	O	106	ASN
2	O	118	HIS
1	F	153	HIS
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	277	ASN
1	F	304	GLN
1	F	353	HIS
1	F	386	HIS
1	F	401	GLN
1	F	420	ASN
2	K	106	ASN
2	K	118	HIS
1	G	153	HIS
1	G	156	GLN
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	277	ASN
1	G	304	GLN
1	G	353	HIS
1	G	383	HIS
1	G	386	HIS
1	G	401	GLN
1	G	420	ASN
2	P	106	ASN
2	P	118	HIS
1	H	123	ASN
1	H	153	HIS
1	H	229	GLN

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Mol	Chain	Res	Type
1	H	238	HIS
1	H	241	ASN
1	H	277	ASN
1	H	304	GLN
1	H	353	HIS
1	H	383	HIS
1	H	386	HIS
1	H	401	GLN
1	H	420	ASN
2	L	106	ASN
2	L	118	HIS

### 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 ⓘ

8 ligands are modelled in this entry.

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	$\# Z  > 2$
3	XBP	A	476	-	17,17,17	2.06	5 (29%)	25,25,25	1.49	4 (16%)
3	XBP	B	476	-	17,17,17	2.07	5 (29%)	25,25,25	1.49	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XBP	C	476	-	17,17,17	2.07	5 (29%)	25,25,25	1.49	4 (16%)
3	XBP	D	476	-	17,17,17	2.07	5 (29%)	25,25,25	1.48	4 (16%)
3	XBP	E	476	-	17,17,17	2.07	5 (29%)	25,25,25	1.49	4 (16%)
3	XBP	F	476	1	17,17,17	2.07	5 (29%)	25,25,25	1.48	4 (16%)
3	XBP	G	476	1	17,17,17	2.05	5 (29%)	25,25,25	1.49	4 (16%)
3	XBP	H	476	-	17,17,17	2.06	5 (29%)	25,25,25	1.49	4 (16%)

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
3	XBP	A	476	-	-	0/20/20/20	0/0/0/0
3	XBP	B	476	-	-	0/20/20/20	0/0/0/0
3	XBP	C	476	-	-	0/20/20/20	0/0/0/0
3	XBP	D	476	-	-	0/20/20/20	0/0/0/0
3	XBP	E	476	-	-	0/20/20/20	0/0/0/0
3	XBP	F	476	1	-	0/20/20/20	0/0/0/0
3	XBP	G	476	1	-	0/20/20/20	0/0/0/0
3	XBP	H	476	-	-	0/20/20/20	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	476	XBP	O1-C1	5.54	1.47	1.43
3	F	476	XBP	O1-C1	5.49	1.46	1.43
3	D	476	XBP	O1-C1	5.48	1.46	1.43
3	B	476	XBP	O1-C1	5.47	1.46	1.43
3	C	476	XBP	O1-C1	5.43	1.46	1.43
3	H	476	XBP	O1-C1	5.42	1.46	1.43
3	A	476	XBP	O1-C1	5.41	1.46	1.43
3	G	476	XBP	O1-C1	5.38	1.46	1.43
3	G	476	XBP	P2-O5	-3.27	1.48	1.60
3	B	476	XBP	P2-O5	-3.24	1.48	1.60
3	D	476	XBP	P2-O5	-3.23	1.48	1.60
3	H	476	XBP	P2-O5	-3.23	1.48	1.60
3	F	476	XBP	P2-O5	-3.23	1.48	1.60
3	A	476	XBP	P2-O5	-3.23	1.48	1.60
3	C	476	XBP	P2-O5	-3.22	1.49	1.60
3	E	476	XBP	P2-O5	-3.16	1.49	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	476	XBP	P1-O1	-2.49	1.51	1.60
3	D	476	XBP	P1-O1	-2.49	1.51	1.60
3	C	476	XBP	P1-O1	-2.48	1.51	1.60
3	E	476	XBP	P1-O1	-2.48	1.51	1.60
3	F	476	XBP	P1-O1	-2.48	1.51	1.60
3	A	476	XBP	P1-O1	-2.47	1.51	1.60
3	G	476	XBP	P1-O1	-2.47	1.51	1.60
3	H	476	XBP	P1-O1	-2.46	1.51	1.60
3	D	476	XBP	P1-O1P	2.38	1.59	1.51
3	G	476	XBP	P1-O1P	2.38	1.59	1.51
3	F	476	XBP	P1-O1P	2.37	1.59	1.51
3	C	476	XBP	P1-O1P	2.37	1.59	1.51
3	B	476	XBP	P1-O1P	2.36	1.59	1.51
3	A	476	XBP	P1-O1P	2.36	1.59	1.51
3	H	476	XBP	P1-O1P	2.35	1.59	1.51
3	E	476	XBP	P1-O1P	2.31	1.59	1.51
3	D	476	XBP	P2-O6P	2.17	1.62	1.54
3	C	476	XBP	P2-O6P	2.17	1.62	1.54
3	G	476	XBP	P2-O6P	2.17	1.62	1.54
3	H	476	XBP	P2-O6P	2.17	1.62	1.54
3	F	476	XBP	P2-O6P	2.17	1.62	1.54
3	A	476	XBP	P2-O6P	2.16	1.62	1.54
3	E	476	XBP	P2-O6P	2.16	1.62	1.54
3	B	476	XBP	P2-O6P	2.14	1.62	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	476	XBP	P2-O5-C5	3.69	128.86	118.19
3	H	476	XBP	P2-O5-C5	3.67	128.81	118.19
3	C	476	XBP	P2-O5-C5	3.67	128.82	118.19
3	F	476	XBP	P2-O5-C5	3.67	128.80	118.19
3	D	476	XBP	P2-O5-C5	3.67	128.79	118.19
3	A	476	XBP	P2-O5-C5	3.66	128.78	118.19
3	B	476	XBP	P2-O5-C5	3.66	128.77	118.19
3	G	476	XBP	P2-O5-C5	3.64	128.72	118.19
3	G	476	XBP	O1-C1-C2	2.58	114.41	110.31
3	C	476	XBP	O1-C1-C2	2.56	114.37	110.31
3	B	476	XBP	O1-C1-C2	2.55	114.36	110.31
3	H	476	XBP	O1-C1-C2	2.54	114.35	110.31
3	A	476	XBP	O1-C1-C2	2.53	114.33	110.31
3	D	476	XBP	O1-C1-C2	2.53	114.33	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	476	XBP	O1-C1-C2	2.52	114.32	110.31
3	E	476	XBP	O1-C1-C2	2.50	114.28	110.31
3	C	476	XBP	C1-C2-C3	2.10	120.14	116.33
3	G	476	XBP	C1-C2-C3	2.10	120.14	116.33
3	H	476	XBP	C1-C2-C3	2.09	120.12	116.33
3	B	476	XBP	C1-C2-C3	2.09	120.11	116.33
3	A	476	XBP	C1-C2-C3	2.07	120.09	116.33
3	D	476	XBP	C1-C2-C3	2.06	120.07	116.33
3	F	476	XBP	C1-C2-C3	2.05	120.05	116.33
3	E	476	XBP	O5-C5-C4	2.05	122.52	105.77
3	B	476	XBP	O5-C5-C4	2.04	122.40	105.77
3	D	476	XBP	O5-C5-C4	2.04	122.39	105.77
3	F	476	XBP	O5-C5-C4	2.04	122.39	105.77
3	A	476	XBP	O5-C5-C4	2.04	122.39	105.77
3	H	476	XBP	O5-C5-C4	2.03	122.38	105.77
3	C	476	XBP	O5-C5-C4	2.03	122.38	105.77
3	E	476	XBP	C1-C2-C3	2.03	120.02	116.33
3	G	476	XBP	O5-C5-C4	2.03	122.30	105.77

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.