Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 05:17 am BST

PDB ID	:	1RSC
Title	:	STRUCTURE OF AN EFFECTOR INDUCED INACTIVATED STATE OF RIBULOSE BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE : THE BINARY COMPLEX BETWEEN ENZYME AND XYLULOSE BISPHOSPHATE
Authors	:	Newman, J.; Gutteridge, S.
Deposited on	:	1994-03-29
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

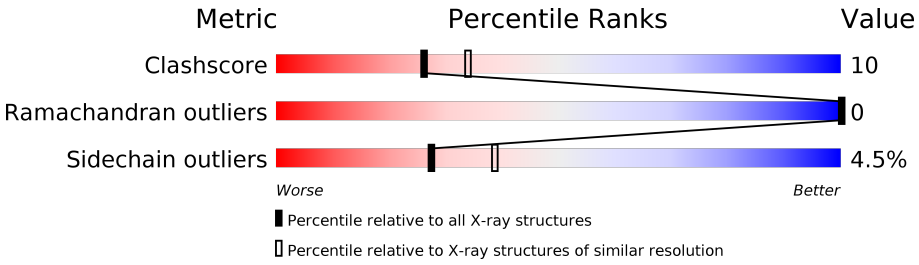
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	75% 21%
1	B	472	75% 21%
1	C	472	74% 22%
1	D	472	76% 20%
1	E	472	74% 22%
1	F	472	73% 23%
1	G	472	74% 22%
1	H	472	73% 23%

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Mol	Chain	Length	Quality of chain
2	I	111	77% 22%
2	J	111	76% 23%
2	K	111	79% 19%
2	L	111	77% 22%
2	M	111	74% 24%
2	N	111	79% 19%
2	O	111	74% 24%
2	P	111	75% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 36846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (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 BISPHOSPHATE CARBOXYLASE/OXYGENASE (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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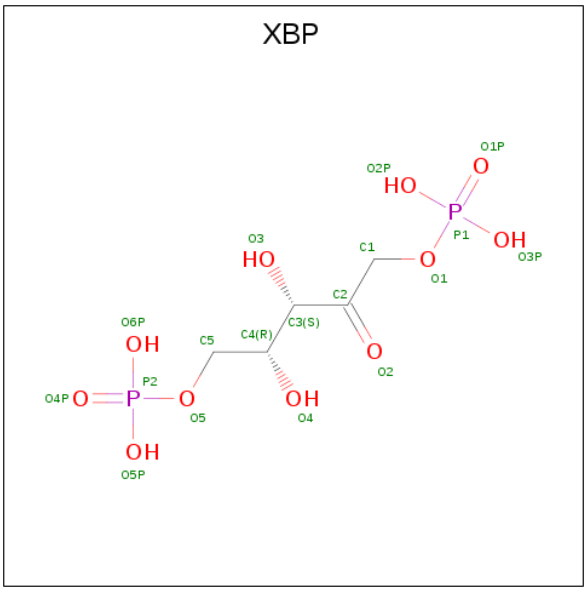
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	P	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			
2	L	109	Total	C	N	O	S	58	0	0
			909	583	154	165	7			

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 XYLULOSE-1,5-BISPHOSPHATE (three-letter code: XBP) (formula: $C_5H_{12}O_{11}P_2$).



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	C	O	P	0	0
			18	5	11	2		
3	D	1	Total	C	O	P	0	0
			18	5	11	2		
3	E	1	Total	C	O	P	0	0
			18	5	11	2		
3	F	1	Total	C	O	P	0	0
			18	5	11	2		
3	G	1	Total	C	O	P	0	0
			18	5	11	2		
3	H	1	Total	C	O	P	0	0
			18	5	11	2		

- Molecule 4 is water.

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

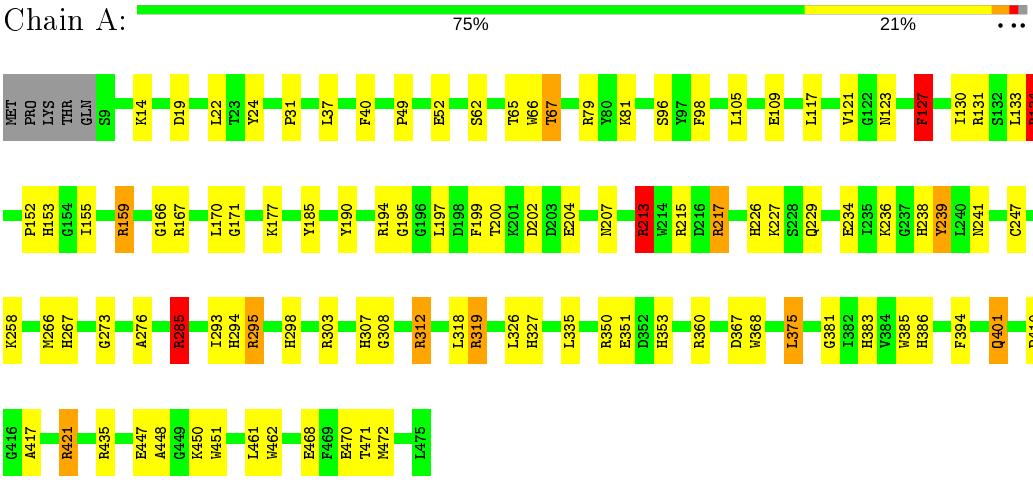
3 Residue-property plots (i)

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

Note EDS was not executed.

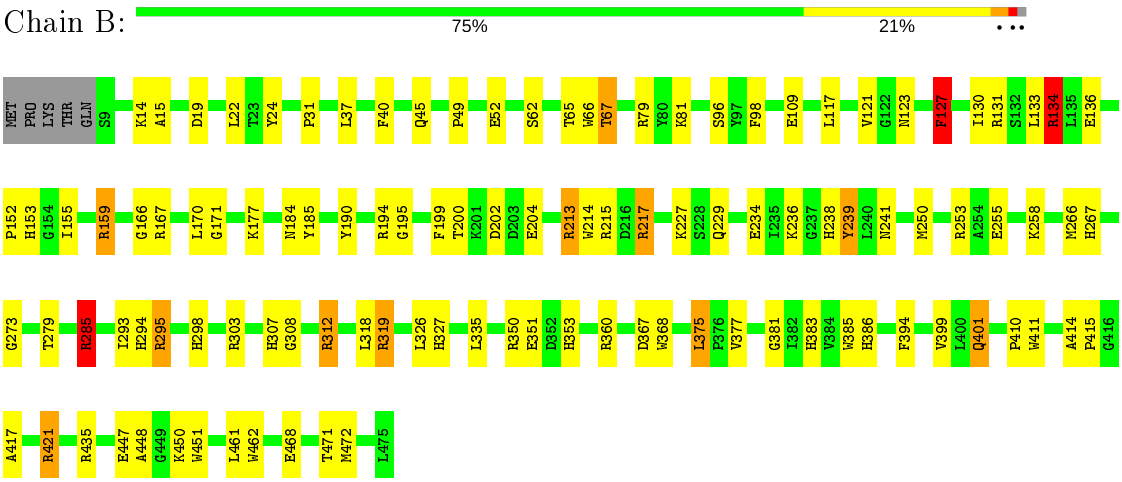
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain A:



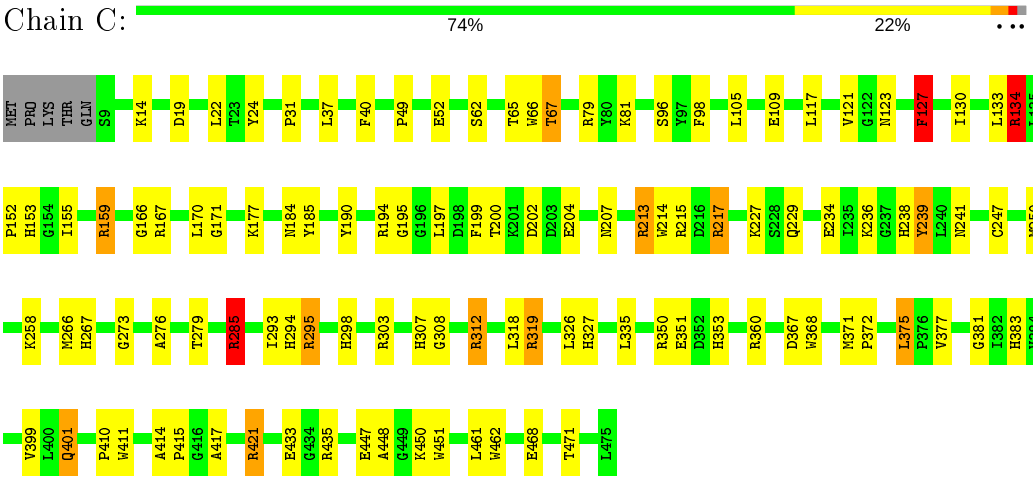
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain B:



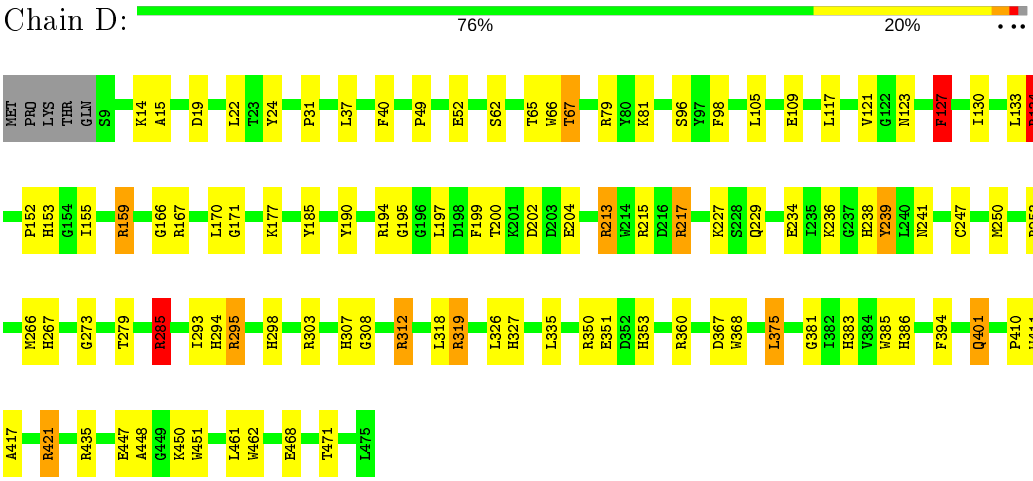
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain C:



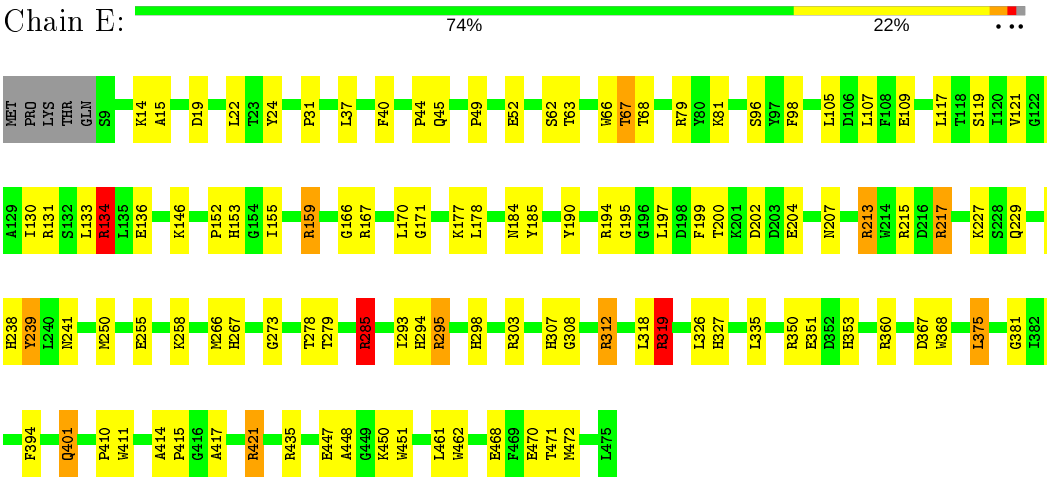
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain D:



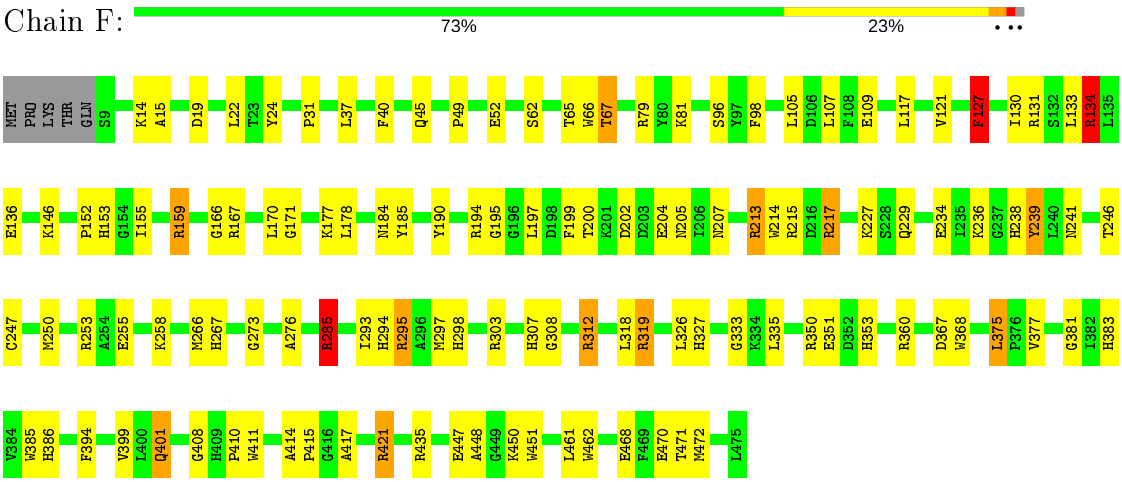
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain E:



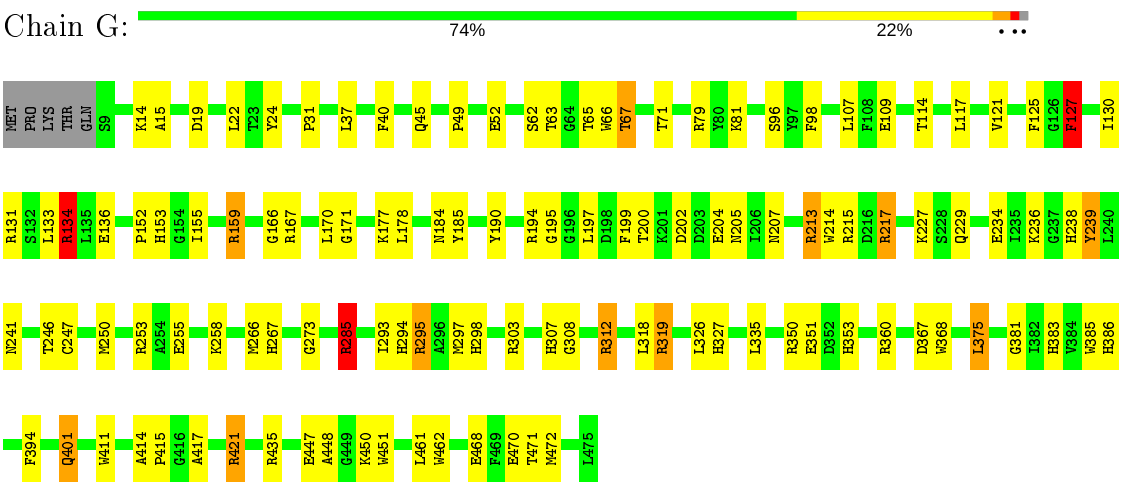
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain F:



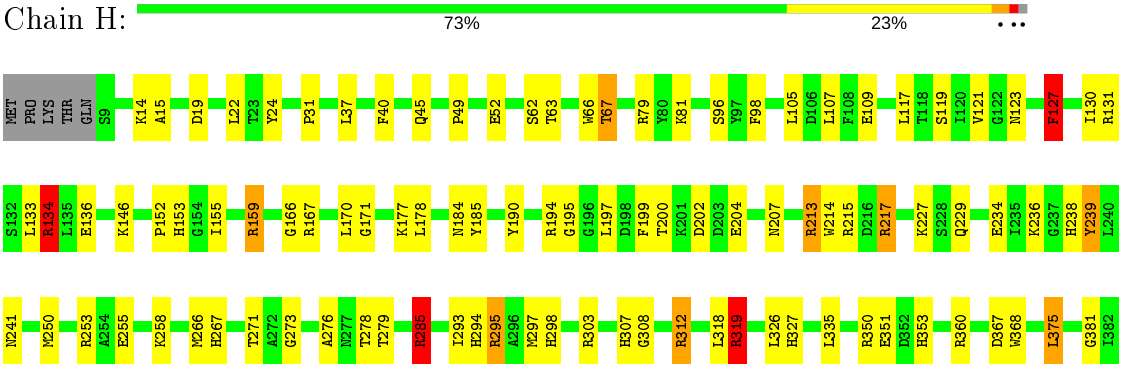
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain G:



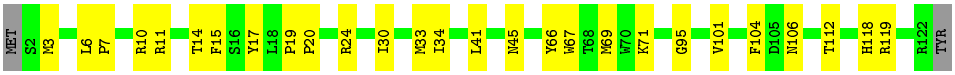
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain H:



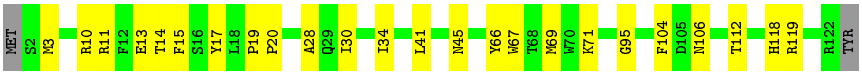
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain M:



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

Chain I:



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

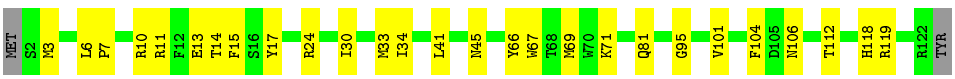
Chain N:

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

Chain J:

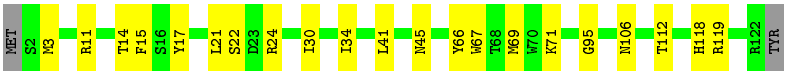
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain O:



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

Chain K:

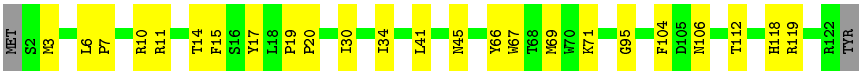


• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain P:

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

Chain L:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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^2)	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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:MET:HE2	1:D:267:HIS:NE2	2.05	0.72
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:B:250:MET:HE2	1:B:267:HIS:NE2	2.04	0.71
1:E:250:MET:HE2	1:E: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:A:250:MET:HE1	1:A:267:HIS:CE1	2.28	0.69
1:G:335:LEU:HD23	1:H:127:PHE:CD1	2.26	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:E:234:GLU:OE1	1:E:421:ARG:NH2	2.27	0.67
1:H:234:GLU:OE1	1:H: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:A:383:HIS:H	1:A:386:HIS:HD2	1.44	0.66
1:D:383:HIS:H	1:D: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:D:155:ILE:HG12	1:D:375:LEU:HD13	1.78	0.65
1:E:155:ILE:HG12	1:E:375:LEU:HD13	1.79	0.65
1:H:383:HIS:H	1:H:386:HIS:HD2	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:ILE:HG12	1:H:375:LEU:HD13	1.78	0.65
2:P:30:ILE:O	2:P:34:ILE:HG12	1.97	0.65
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:A:335:LEU:CD2	1:B:127:PHE:CD1	2.82	0.63
1:G:381:GLY:HA2	1:H:66:TRP:CD1	2.33	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:A:350:ARG:NH2	1:A:394:PHE:O	2.34	0.61
1:G:350:ARG:NH2	1:G: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:B:350:ARG:NH2	1:B:394:PHE:O	2.34	0.60
1:E:127:PHE:CD1	1:F:335:LEU:HD23	2.37	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:130:ILE:O	1:H:303:ARG:NH2	2.36	0.58
1:G:470:GLU:O	1:H:45:GLN:NE2	2.37	0.58
1:G:107:LEU:HD22	1:H:178:LEU:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:229:GLN:NE2	1:A:236:LYS:H	2.03	0.56
1:C:229:GLN:NE2	1:C:236:LYS:H	2.03	0.56
1:B:411:TRP:CD1	2:I:3:MET:HB3	2.41	0.56
1:E:335:LEU:HD23	1:F:127:PHE:CD1	2.39	0.56
1:E:234:GLU:CD	1:E:421:ARG:HH22	2.09	0.56
1:H:411:TRP:CD1	2:L:3:MET:HB3	2.41	0.56
1:D:318:LEU:O	1:D:318:LEU:HG	2.06	0.56
1:D:411:TRP:CD1	2:J:3:MET:HB3	2.41	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:A:319:ARG:NH2	1:A:351:GLU:O	2.35	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:H:229:GLN:NE2	1:H:236:LYS:H	2.03	0.56
1:B:318:LEU:HG	1:B:318:LEU:O	2.06	0.56
1:C:127:PHE:CD1	1:D:335:LEU:CD2	2.89	0.56
1:H:234:GLU:CD	1:H:421:ARG:HH22	2.10	0.56
1:A:250:MET:HE2	1:A:267:HIS:NE2	2.21	0.55
1:C:318:LEU:O	1:C:318:LEU:HG	2.06	0.55
1:E:127:PHE:HD1	1:F:335:LEU:CD2	2.17	0.55
1:B:234:GLU:CD	1:B:421:ARG:HH22	2.10	0.55
1:A:123:ASN:ND2	1:B:204:GLU:OE2	2.39	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: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:127:PHE:CD1	1:B:335:LEU:HD21	2.42	0.55
1:A:335:LEU:HD23	1:B:127:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:TRP:CD1	2:P:3:MET:HB3	2.41	0.55
1:B:319:ARG:NH2	1:B:351:GLU:O	2.35	0.55
1:F:234:GLU:CD	1:F:421:ARG:HH22	2.10	0.55
1:A:318:LEU:O	1:A:318:LEU:HG	2.06	0.55
1:D:234:GLU:CD	1:D:421:ARG:HH22	2.10	0.55
1:E:62:SER:O	1:F:177:LYS:HB2	2.07	0.55
1:G:127:PHE:CD1	1:H:335:LEU:HD21	2.42	0.55
1:H:318:LEU:O	1:H:318:LEU:HG	2.06	0.55
1:A:381:GLY:HA2	1:B:66:TRP:CD1	2.42	0.54
1:D:250:MET:HE2	1:D:267:HIS:CD2	2.43	0.54
1:G:67:THR:CG2	1:H:462:TRP:HE1	1.95	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:A:234:GLU:CD	1:A:421:ARG:HH22	2.09	0.54
1:E:250:MET:CE	1:E:267:HIS:CE1	2.91	0.54
1:G:318:LEU:HG	1:G:318:LEU:O	2.06	0.54
1:G:472:MET:HG3	1:H:131:ARG:O	2.07	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:E:318:LEU:HG	1:E:318:LEU:O	2.06	0.54
1:G:127:PHE:HD1	1:H:335:LEU:CD2	2.18	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
1:G:109:GLU:OE1	1:H:207:ASN:HB3	2.08	0.53
2:O:104:PHE:HZ	1:G:184:ASN:HD21	1.55	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:E:319:ARG:NH2	1:E:351:GLU:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:LEU:HD21	1:H:127:PHE:CE1	2.45	0.51
1:A:213:ARG:HD2	4:A:491:HOH:O	2.10	0.51
1:E:295:ARG:HD2	1:E:327:HIS:HB2	1.93	0.51
1:H:31:PRO:HB3	1:H:37:LEU:HD21	1.93	0.51
1:A:31:PRO:HB3	1:A:37:LEU:HD21	1.93	0.51
1:E:335:LEU:HD21	1:F:127:PHE:CD1	2.45	0.51
2:N:104:PHE:HZ	1:E:184:ASN:HD21	1.56	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:G:66:TRP:CH2	1:H:383:HIS:CD2	2.99	0.51
1:D:31:PRO:HB3	1:D:37:LEU:HD21	1.93	0.51
1:F:31:PRO:HB3	1:F:37:LEU:HD21	1.93	0.51
1:C:31:PRO:HB3	1:C: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:E:202:ASP:OD1	1:E:238:HIS:HE1	1.94	0.51
1:E:448:ALA:HA	1:E:451:TRP:NE1	2.26	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:A:295:ARG:HD2	1:A:327:HIS:HB2	1.93	0.50
1:B:295:ARG:HD2	1:B:327:HIS:HB2	1.93	0.50
1:B:31:PRO:HB3	1:B:37:LEU:HD21	1.93	0.50
1:C:295:ARG:HD2	1:C:327:HIS:HB2	1.93	0.50
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.94	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:F:250:MET:CE	1:F:267:HIS:HE2	2.23	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:B:448:ALA:HA	1:B:451:TRP:NE1	2.26	0.50
1:F:448:ALA:HA	1:F:451:TRP:NE1	2.26	0.50
1:G:448:ALA:HA	1:G:451:TRP:NE1	2.27	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:F:295:ARG:HD2	1:F:327:HIS:HB2	1.93	0.50
1:E:414:ALA:HB3	1:E:415:PRO:HD3	1.94	0.50
1:H:295:ARG:HD2	1:H:327:HIS:HB2	1.93	0.50
1:H:448:ALA:HA	1:H:451:TRP:NE1	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:LEU:HD21	1:F:15:ALA:HB1	1.93	0.50
1:A:448:ALA:HA	1:A:451:TRP:NE1	2.26	0.50
1:B:250:MET:HE2	1:B:267:HIS:CD2	2.46	0.50
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.94	0.50
1:F:184:ASN:HD21	2:L:104:PHE:HZ	1.57	0.50
1:G:250:MET:HE2	1:G:267:HIS:CD2	2.47	0.50
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.94	0.49
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:A:435:ARG:NH2	1:A:447:GLU:OE1	2.45	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
2:O:69:MET:HE3	2:O:71:LYS:O	2.13	0.49
1:C:435:ARG:NH2	1:C:447:GLU:OE1	2.45	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:G:295:ARG:HD2	1:G:327:HIS:HB2	1.93	0.49
1:C:414:ALA:HB3	1:C:415:PRO:HD3	1.95	0.49
1:D:435:ARG:NH2	1:D:447:GLU:OE1	2.45	0.49
1:E:109:GLU:OE2	1:F:253:ARG:NH2	2.28	0.49
1:H:435:ARG:NH2	1:H:447:GLU:OE1	2.45	0.49
1:A:335:LEU:CD2	1:B:127:PHE:HD1	2.25	0.49
1:B:250:MET:CE	1:B:267:HIS:HE2	2.23	0.49
1:C:117:LEU:O	1:C:121:VAL:HG22	2.13	0.49
1:E:435:ARG:NH2	1:E:447:GLU:OE1	2.46	0.49
1:F:117:LEU:O	1:F:121:VAL:HG22	2.13	0.49
1:B:117:LEU:O	1:B:121:VAL:HG22	2.13	0.49
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.94	0.49
1:D:250:MET:HE1	1:D:267:HIS:CE1	2.47	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: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:40:PHE:O	1:A:98:PHE:HA	2.13	0.49
1:B:435:ARG:NH2	1:B:447:GLU:OE1	2.45	0.49
1:A:67:THR:CG2	1:B:462:TRP:HE1	2.02	0.49
1:C:204:GLU:OE2	1:D:123:ASN:ND2	2.46	0.49
1:E:177:LYS:HB2	1:F:62:SER:O	2.13	0.49
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.96	0.49
1:H:250:MET:CE	1:H:267:HIS:HE2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:117:LEU:O	1:A:121:VAL:HG22	2.13	0.48
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.94	0.48
1:D:40:PHE:O	1:D:98:PHE:HA	2.13	0.48
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.96	0.48
1:G:125:PHE:O	1:H:303:ARG:HD3	2.13	0.48
1:A:461:LEU:HD21	1:B:15:ALA:HB1	1.93	0.48
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: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
1:G:178:LEU:HD12	1:H:107:LEU:HD22	1.94	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
2:J:69:MET:HE3	2:J:71:LYS:O	2.13	0.48
1:F:229:GLN:HE21	1:F:236:LYS:H	1.62	0.48
1:H:250:MET:HE2	1:H:267:HIS:CD2	2.48	0.48
1:A:319:ARG:HG2	1:A: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:E:319:ARG:HG2	1:E:368:TRP:CZ3	2.49	0.48
1:G:318:LEU:HD22	1:G:326:LEU:HD13	1.96	0.48
1:H:117:LEU:O	1:H:121:VAL:HG22	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:C:295:ARG:HG3	1:C:298:HIS:CD2	2.49	0.48
1:D:117:LEU:O	1:D:121:VAL:HG22	2.13	0.48
1:E:295:ARG:HG3	1:E:298:HIS:CD2	2.49	0.48
2:N:69:MET:HE3	2:N:71:LYS:O	2.14	0.48
1:E:134:ARG:HA	1:E:308:GLY:O	2.14	0.48
1:E:250:MET:HE1	1:E:267:HIS:CE1	2.49	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:250:MET:CE	1:G:267:HIS:HE2	2.24	0.48
1:G:40:PHE:O	1:G:98:PHE:HA	2.13	0.48
2:P:69:MET:HE3	2:P:72:LEU:HD23	1.95	0.48
1:A:472:MET:HG3	1:B:131:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ARG:HG3	1:B:298:HIS:CD2	2.49	0.48
1:C:319:ARG:HG2	1:C:368:TRP:CZ3	2.49	0.48
1:G:414:ALA:HB3	1:G:415:PRO:HD3	1.95	0.48
2:I:69:MET:HE3	2:I:71:LYS:O	2.14	0.48
2:L:69:MET:HE3	2:L:71:LYS:O	2.14	0.48
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.96	0.47
1:A:247:CYS:H	1:B:279:THR:HG1	1.62	0.47
1:B:134:ARG:HA	1:B:308:GLY:O	2.14	0.47
1:C:109:GLU:OE2	1:D:253:ARG:NH2	2.32	0.47
1:C:318:LEU:HD22	1:C:326:LEU:HD13	1.96	0.47
1:G:295:ARG:HG3	1:G:298:HIS:CD2	2.49	0.47
1:G:204:GLU:OE2	1:H:123:ASN:ND2	2.47	0.47
1:H:295:ARG:HG3	1:H:298:HIS:CD2	2.49	0.47
1:A:146:LYS:HD2	1:D:105:LEU:HD21	1.96	0.47
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.49	0.47
1:B:49:PRO:HG2	1:B:52:GLU:HB3	1.96	0.47
1:A:177:LYS:HB2	1:B:62:SER:O	2.14	0.47
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.96	0.47
1:C:250:MET:CE	1:C:267:HIS:HE2	2.23	0.47
1:C:49:PRO:HG2	1:C:52:GLU:HB3	1.96	0.47
1:D:134:ARG:HA	1:D:308:GLY:O	2.14	0.47
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.96	0.47
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.96	0.47
1:E:49:PRO:HG2	1:E:52:GLU:HB3	1.96	0.47
1:H:319:ARG:HG2	1:H:368:TRP:CZ3	2.49	0.47
1:A:250:MET:CE	1:A:267:HIS:HE2	2.23	0.47
3:C:476:XBP:O2P	1:D:65:THR:OG1	2.22	0.47
1:D:19:ASP:HB2	1:D:22:LEU:HG	1.97	0.47
1:G:134:ARG:HA	1:G:308:GLY:O	2.15	0.47
1:H:250:MET:HE2	1:H:267:HIS:CE1	2.50	0.47
2:N:119:ARG:HG3	2:N:119:ARG:HH11	1.79	0.47
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.49	0.47
1:A:318:LEU:HD22	1:A:326:LEU:HD13	1.96	0.47
1:C:335:LEU:HD21	1:D:127:PHE:CD1	2.50	0.47
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.49	0.47
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.49	0.47
1:F:295:ARG:HG3	1:F:298: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
2:M:69:MET:HE3	2:M:71:LYS:O	2.14	0.47
1:B:318:LEU:HD22	1:B:326:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:49:PRO:HG2	1:H:52:GLU:HB3	1.96	0.47
1:A:19:ASP:HB2	1:A:22:LEU:HG	1.96	0.47
1:G:166:GLY:HA2	2:P:112:THR:O	2.15	0.47
1:A:447:GLU:O	1:A:450:LYS:HB2	2.15	0.47
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.49	0.47
1:C:134:ARG:HA	1:C:308:GLY:O	2.14	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
1:E:318:LEU:HD22	1:E:326:LEU:HD13	1.96	0.47
1:F:318:LEU:HD22	1:F:326:LEU:HD13	1.96	0.47
1:H:229:GLN:HE21	1:H:236:LYS:H	1.62	0.47
2:L:119:ARG:HG3	2:L:119:ARG:HH11	1.79	0.47
1:A:49:PRO:HG2	1:A:52:GLU:HB3	1.96	0.47
1:D:447:GLU:O	1:D:450:LYS:HB2	2.15	0.47
1:E:66:TRP:CD1	1:F:381:GLY:HA2	2.50	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
2:I:119:ARG:HH11	2:I:119:ARG:HG3	1.79	0.47
1:H:166:GLY:HA2	2:L:112:THR:O	2.15	0.47
1:B:229:GLN:HE21	1:B:236:LYS:H	1.62	0.47
1:C:19:ASP:HB2	1:C:22:LEU:HG	1.96	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:G:319:ARG:HG2	1:G:368:TRP:CZ3	2.49	0.47
1:B:166:GLY:HA2	2:I:112:THR:O	2.15	0.47
1:G:185:TYR:OH	1:G:202:ASP:HA	2.15	0.47
1:G:229:GLN:HE21	1:G:236:LYS:H	1.62	0.47
1:G:49:PRO:HG2	1:G:52:GLU:HB3	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:A:130:ILE:O	1:B:303:ARG:NH2	2.44	0.47
1:B:447:GLU:O	1:B:450:LYS:HB2	2.15	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:E:447:GLU:O	1:E:450:LYS:HB2	2.15	0.47
1:G:19:ASP:HB2	1:G:22:LEU:HG	1.96	0.47
1:A:134:ARG:HA	1:A:308:GLY:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.49	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:H:159:ARG:NH2	1:H:167:ARG:O	2.47	0.46
2:O:119:ARG:HH11	2:O:119:ARG:HG3	1.79	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:C:166:GLY:HA2	2:N:112:THR:O	2.15	0.46
1:E:166:GLY:HA2	2:O:112:THR:O	2.15	0.46
1:E:207:ASN:HB3	1:F:109:GLU:OE1	2.15	0.46
2:P:119:ARG:HH11	2:P:119:ARG:HG3	1.80	0.46
1:E:185:TYR:OH	1:E:202:ASP:HA	2.16	0.46
1:E:229:GLN:HE21	1:E:236:LYS:H	1.62	0.46
2:J:119:ARG:HG3	2:J:119:ARG:HH11	1.79	0.46
1:A:166:GLY:HA2	2:M:112:THR:O	2.15	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: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:H:318:LEU:HD22	1:H:326:LEU:HD13	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:A:185:TYR:OH	1:A:202:ASP:HA	2.16	0.46
1:C:335:LEU:HD23	1:D:127:PHE:CD1	2.50	0.46
1:D:49:PRO:HG2	1:D:52:GLU:HB3	1.96	0.46
1:F:250:MET:HE1	1:F:276:ALA:HB1	1.97	0.46
1:H:185:TYR:OH	1:H:202:ASP:HA	2.16	0.46
1:B:185:TYR:OH	1:B:202:ASP:HA	2.16	0.45
1:C:447:GLU:O	1:C:450:LYS:HB2	2.15	0.45
1:G:383:HIS:HD2	1:H:66:TRP:CH2	2.34	0.45
1:D:166:GLY:HA2	2:J:112:THR:O	2.15	0.45
1:C:66:TRP:CD1	1:D:381:GLY:HA2	2.51	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:A:295:ARG:HG3	1:A:298:HIS:CG	2.52	0.45
1:E:295:ARG:HG3	1:E:298:HIS:CG	2.52	0.45
1:F:295:ARG:HG3	1:F:298:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:LEU:HD13	1:H:107:LEU:HD22	1.98	0.45
1:A:204:GLU:OE2	1:B:123:ASN:ND2	2.50	0.45
1:E:383:HIS:HD2	1:F:66:TRP:CH2	2.35	0.45
1:B:295:ARG:HG3	1:B:298:HIS:CG	2.52	0.45
1:D:295:ARG:HG3	1:D: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:B:293:ILE:HG21	1:B:318:LEU:HD13	1.99	0.44
1:G:295:ARG:HG3	1:G:298:HIS:CG	2.52	0.44
1:G:293:ILE:HG21	1:G:318:LEU:HD13	1.99	0.44
1:A:293:ILE:HG21	1:A:318:LEU:HD13	1.99	0.44
1:E:250:MET:CE	1:E:267:HIS:HE2	2.23	0.44
1:H:295:ARG:HG3	1:H:298:HIS:CG	2.52	0.44
1:A:105:LEU:HD21	1:D:146:LYS:HD2	1.99	0.44
1:E:293:ILE:HG21	1:E:318:LEU:HD13	2.00	0.44
1:F:293:ILE:HG21	1:F:318:LEU:HD13	1.99	0.44
1:A:250:MET:HE3	1:A:276:ALA:HB1	2.00	0.44
1:C:293:ILE:HG21	1:C:318:LEU:HD13	1.99	0.44
1:C:127:PHE:CD1	1:D:335:LEU:HD23	2.52	0.44
1:G:66:TRP:CG	1:H:381:GLY:HA2	2.52	0.44
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.66	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: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:383:HIS:CE1	1:H:385:TRP:HB2	2.53	0.44
1:A:159:ARG:NH2	1:A:167:ARG:O	2.47	0.44
1:C:152:PRO:O	1:C:285:ARG:HD3	2.18	0.44
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.66	0.44
1:G:383:HIS:CE1	1:G:385:TRP:HB2	2.53	0.44
1:G:207:ASN:HB3	1:H:109:GLU:OE1	2.18	0.44
1:H:130:ILE:HD13	1:H:130:ILE:HA	1.86	0.44
2:O:14:THR:O	2:O:15:PHE:HB2	2.18	0.44
1:A:195:GLY:HA3	1:A:417:ALA:HB3	2.00	0.44
1:B:383:HIS:CE1	1:B:385:TRP:HB2	2.53	0.44
1:C:383:HIS:CE1	1:C:385:TRP:HB2	2.53	0.44
1:D:152:PRO:O	1:D:285:ARG:HD3	2.18	0.44
1:D:383:HIS:CE1	1:D:385:TRP:HB2	2.53	0.44
1:F:383:HIS:CE1	1:F:385:TRP:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:GLY:HA3	1:F:417:ALA:HB3	2.00	0.44
1:G:152:PRO:O	1:G:285:ARG:HD3	2.18	0.44
1:B:159:ARG:NH2	1:B:167:ARG:O	2.47	0.43
1:A:131:ARG:O	1:B:472:MET:HG3	2.18	0.43
1:E:178:LEU:CD1	1:F:107:LEU:HD22	2.48	0.43
1:F:152:PRO:O	1:F:285:ARG:HD3	2.18	0.43
1:B:152:PRO:O	1:B:285:ARG:HD3	2.18	0.43
1:C:130:ILE:HD13	1:C:130:ILE:HA	1.86	0.43
1:C:293:ILE:HG21	1:C:318:LEU:CD1	2.49	0.43
1:D:159:ARG:NH2	1:D:167:ARG:O	2.47	0.43
1:E:470:GLU:O	1:F:45:GLN:NE2	2.50	0.43
1:A:293:ILE:HG21	1:A:318:LEU:CD1	2.49	0.43
1:A:383:HIS:CE1	1:A:385:TRP:HB2	2.53	0.43
1:A:62:SER:O	1:B:177:LYS:HB2	2.18	0.43
1:B:293:ILE:HG21	1:B: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:D:195:GLY:HA3	1:D:417:ALA:HB3	2.00	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
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
1:G:114:THR:HG23	1:H:271:THR:C	2.39	0.43
2:J:14:THR:O	2:J:15:PHE:HB2	2.19	0.43
1:C:239:TYR:HB3	1:C:266:MET:HB2	2.01	0.43
1:H:152:PRO:O	1:H:285:ARG:HD3	2.18	0.43
2:J:11:ARG:HG3	2:J:17:TYR:CE1	2.54	0.43
2:K:14:THR:O	2:K:15:PHE:HB2	2.19	0.43
2:L:14:THR:O	2:L:15:PHE:HB2	2.19	0.43
2:O:6:LEU:HA	2:O:7:PRO:HD3	1.92	0.43
1:B:239:TYR:HB3	1:B:266:MET:HB2	2.01	0.43
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.54	0.43
1:C:195:GLY:HA3	1:C:417:ALA:HB3	2.00	0.43
1:E:128:LYS:HD2	1:F:333:GLY:O	2.18	0.43
1:E:195:GLY:HA3	1:E:417:ALA:HB3	2.00	0.43
1:E:279:THR:HG1	1:F:247:CYS:H	1.67	0.43
2:I:19:PRO:HA	2:I:20:PRO:HD3	1.90	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
1:G:195:GLY:HA3	1:G:417:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:ARG:HG3	2:I:17:TYR:CE1	2.54	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:P:19:PRO:HA	2:P:20:PRO:HD3	1.91	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: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:B:195:GLY:HA3	1:B:417:ALA:HB3	2.00	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:D:171:GLY:HA2	1:D:199:PHE:O	2.19	0.42
1:D:204:GLU:OE1	1:D:294:HIS:CE1	2.72	0.42
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.66	0.42
1:H:293:ILE:HG21	1:H:318:LEU:CD1	2.49	0.42
2:I:14:THR:O	2:I:15:PHE:HB2	2.19	0.42
1:A:383:HIS:HD2	1:B:66:TRP:CH2	2.37	0.42
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.66	0.42
1:B:204:GLU:OE1	1:B:294:HIS:CE1	2.72	0.42
1:C:190:TYR:CZ	1:C:227:LYS:HE3	2.55	0.42
1:E:171:GLY:HA2	1:E:199:PHE:O	2.19	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:G:239:TYR:HE2	1:G:401:GLN:HE22	1.66	0.42
2:L:11:ARG:HG3	2:L: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
1:E:293:ILE:HG21	1:E:318:LEU:CD1	2.49	0.42
1:F:204:GLU:OE1	1:F:294:HIS:CE1	2.72	0.42
1:H:204:GLU:OE1	1:H:294:HIS:CE1	2.72	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
2:O:33:MET:HE1	2:O:101:VAL:HG12	2.01	0.42
2:P:11:ARG:HG3	2:P:17:TYR:CE1	2.54	0.42
1:A:24:TYR:CE1	1:A:81:LYS:HB2	2.55	0.42
1:B:133:LEU:O	1:B:307:HIS:HA	2.20	0.42
1:B:24:TYR:CE1	1:B:81:LYS:HB2	2.55	0.42
1:D:190:TYR:CZ	1:D:227:LYS:HE3	2.55	0.42
1:C:177:LYS:HB2	1:D:62:SER:O	2.20	0.42
1:D:24:TYR:CE1	1:D:81:LYS:HB2	2.55	0.42
1:G:190:TYR:CZ	1:G:227:LYS:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:95:GLY:O	2:O:118:HIS:HE1	2.03	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:C:250:MET:HE2	1:C:267:HIS:CD2	2.53	0.42
1:D:136:GLU:OE1	1:D:312:ARG:NH2	2.53	0.42
1:G:204:GLU:OE1	1:G:294:HIS:CE1	2.72	0.42
1:H:190:TYR:CZ	1:H:227:LYS:HE3	2.55	0.42
1:H:239:TYR:HB3	1:H:266:MET:HB2	2.01	0.42
1:H:24:TYR:CE1	1:H:81:LYS:HB2	2.55	0.42
1:A:136:GLU:OE1	1:A:312:ARG:NH2	2.53	0.42
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.66	0.42
1:C:133:LEU:O	1:C:307:HIS:HA	2.20	0.42
1:E:136:GLU:OE1	1:E:312:ARG:NH2	2.53	0.42
1:E:204:GLU:OE1	1:E:294:HIS:CE1	2.73	0.42
1:G:136:GLU:OE1	1:G:312:ARG:NH2	2.53	0.42
1:G:171:GLY:HA2	1:G:199:PHE:O	2.20	0.42
1:G:71:THR:HG21	1:H:407:LEU:HD23	2.00	0.42
2:I:95:GLY:O	2:I:118:HIS:HE1	2.03	0.42
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:A:470:GLU:O	1:B:45:GLN:NE2	2.53	0.42
1:C:204:GLU:OE1	1:C:294:HIS:CE1	2.72	0.42
1:E:130:ILE:HA	1:E:130:ILE:HD13	1.87	0.42
1:G:24:TYR:CE1	1:G:81:LYS:HB2	2.55	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:A:204:GLU:OE1	1:A:294:HIS:CE1	2.72	0.42
1:B:250:MET:HE1	1:B:267:HIS:CE1	2.55	0.42
1:C:24:TYR:CE1	1:C:81:LYS:HB2	2.55	0.42
1:D:239:TYR:HB3	1:D:266:MET:HB2	2.01	0.42
1:E:410:PRO:HD3	1:E:461:LEU:HD22	2.02	0.42
1:F:171:GLY:HA2	1:F:199:PHE:O	2.20	0.42
1:F:24:TYR:CE1	1:F:81:LYS:HB2	2.55	0.42
2:L:19:PRO:HA	2:L:20:PRO:HD3	1.90	0.42
1:A:190:TYR:CZ	1:A:227:LYS:HE3	2.55	0.42
1:B:171:GLY:HA2	1:B:199:PHE:O	2.19	0.42
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.55	0.42
2:M:104:PHE:HZ	1:C:184:ASN:HD21	1.64	0.42
1:E:133:LEU:O	1:E:307:HIS:HA	2.20	0.42
1:E:178:LEU:HD12	1:F:107:LEU:HD22	2.01	0.42
1:F:136:GLU:OE1	1:F:312:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:LEU:HG	1:G:417:ALA:HB1	2.02	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.20	0.42
1:H:136:GLU:OE1	1:H:312:ARG:NH2	2.53	0.42
1:B:353:HIS:HD2	1:B:367:ASP:OD1	2.03	0.42
1:C:247:CYS:H	1:D:279:THR:HG1	1.67	0.42
1:F:239:TYR:HB3	1:F:266:MET:HB2	2.01	0.42
1:F:197:LEU:HG	1:F:417:ALA:HB1	2.02	0.42
2:J:6:LEU:HA	2:J:7:PRO:HD3	1.92	0.42
2:P:6:LEU:HA	2:P:7:PRO:HD3	1.92	0.42
1:A:133:LEU:O	1:A:307:HIS:HA	2.20	0.41
1:A:239:TYR:HB3	1:A:266:MET:HB2	2.01	0.41
1:E:146:LYS:HD2	1:H:105:LEU:HD21	2.03	0.41
1:G:461:LEU:CD2	1:H:15:ALA:HB1	2.49	0.41
2:J:95:GLY:O	2:J:118:HIS:HE1	2.03	0.41
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.66	0.41
1:E:353:HIS:HD2	1:E:367:ASP:OD1	2.03	0.41
1:F:133:LEU:O	1:F:307:HIS:HA	2.20	0.41
1:F:159:ARG:NH2	1:F:167:ARG:O	2.47	0.41
1:G:239:TYR:HB3	1:G:266:MET:HB2	2.01	0.41
2:K:95:GLY:O	2:K:118:HIS:HE1	2.03	0.41
2:L:95:GLY:O	2:L:118:HIS:HE1	2.03	0.41
2:M:45:ASN:HB2	2:M:67:TRP:CD2	2.55	0.41
1:A:226:HIS:HE1	4:A:487:HOH:O	2.03	0.41
1:C:353:HIS:HD2	1:C:367:ASP:OD1	2.03	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
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: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:D:133:LEU:O	1:D:307:HIS:HA	2.20	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: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
1:D:410:PRO:HD3	1:D:461:LEU:HD22	2.02	0.41
1:G:133:LEU:O	1:G:307:HIS:HA	2.20	0.41
2:M:95:GLY:O	2:M:118:HIS:HE1	2.03	0.41
2:O:10:ARG:O	2:O:11:ARG:HD2	2.21	0.41
1:E:197:LEU:HG	1:E:417:ALA:HB1	2.03	0.41
1:F:353:HIS:HD2	1:F:367:ASP:OD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ARG:NH2	1:G:167:ARG:O	2.47	0.41
1:G:127:PHE:CE1	1:H:335:LEU:HD21	2.56	0.41
1:H:410:PRO:HD3	1:H:461:LEU:HD22	2.02	0.41
2:I:45:ASN:HB2	2:I:67:TRP:CD2	2.56	0.41
2:L:45:ASN:HB2	2:L:67:TRP:CD2	2.55	0.41
2:M:118:HIS:HD2	4:M:155:HOH:O	2.02	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
1:E:24:TYR:CE1	1:E:81:LYS:HB2	2.55	0.41
2:K:45:ASN:HB2	2:K:67:TRP:CD2	2.56	0.41
1:E:15:ALA:HB1	1:F:461:LEU:HD21	2.03	0.41
2:P:95:GLY:O	2:P:118:HIS:HE1	2.03	0.41
1:A:353:HIS:HD2	1:A:367:ASP:OD1	2.03	0.41
1:C:371:MET:HA	1:C:372:PRO:HD3	1.97	0.41
1:D:197:LEU:HG	1:D:417:ALA:HB1	2.02	0.41
1:F:130:ILE:HA	1:F:130:ILE:HD13	1.86	0.41
1:G:247:CYS:H	1:H:279:THR:HG1	1.69	0.41
1:B:250:MET:HE2	1:B:267:HIS:CE1	2.53	0.41
1:C:130:ILE:O	1:D:303:ARG:NH2	2.54	0.41
1:C:159:ARG:NH2	1:C:167:ARG:O	2.47	0.41
1:G:214:TRP:CD2	1:G:253:ARG:HG2	2.56	0.41
2:I:104:PHE:HZ	1:H:184:ASN:HD21	1.63	0.41
1:H:197:LEU:HG	1:H:417:ALA:HB1	2.02	0.41
2:M:6:LEU:HA	2:M:7:PRO:HD3	1.92	0.41
1:A:197:LEU:HG	1:A:417:ALA:HB1	2.02	0.40
1:C:105:LEU:HD21	1:F:146:LYS:HD2	2.03	0.40
1:E:121:VAL:O	1:F:297:MET:HA	2.21	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
1:G:71:THR:CG2	1:H:407:LEU:HD23	2.51	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
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:B:377:VAL:HG22	1:B:399:VAL:HB	2.03	0.40
1:C:279:THR:HG1	1:D:247:CYS:H	1.69	0.40
1:C:146:LYS:HD2	1:F:105:LEU:HD21	2.03	0.40
2:I:10:ARG:O	2:I:11:ARG:HD2	2.21	0.40
2:L:6:LEU:HA	2:L:7:PRO:HD3	1.92	0.40
2:O:13:GLU:HB3	2:O:14:THR:H	1.73	0.40
2:O:45:ASN:HB2	2:O:67:TRP:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:10:ARG:O	2:P:11:ARG:HD2	2.21	0.40
2:P:45:ASN:HB2	2:P:67:TRP:CD2	2.56	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
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:O:11:ARG:HH21	2:O:17:TYR:HA	1.87	0.40
2:P:11:ARG:HH21	2:P:17:TYR:HA	1.87	0.40
1:C:197:LEU:HG	1:C:417:ALA:HB1	2.02	0.40
1:C:303:ARG:NH2	1:D:130:ILE:O	2.54	0.40
1:E:109:GLU:OE1	1:F:207:ASN:HB3	2.21	0.40
1:H:214:TRP:CD2	1:H:253:ARG:HG2	2.57	0.40
2:K:11:ARG:HG3	2:K:17:TYR:CZ	2.57	0.40
1:A:109:GLU:OE2	1:B:253:ARG:NH2	2.35	0.40
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.86	0.40
1:B:214:TRP:CD2	1:B:253:ARG:HG2	2.57	0.40
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
1:E:44:PRO:HA	1:E:130:ILE:HD13	2.03	0.40
1:F:214:TRP:CD2	1:F:253:ARG:HG2	2.57	0.40
1:F:377:VAL:HG22	1:F:399:VAL:HB	2.03	0.40
2:M:10:ARG:O	2:M:11:ARG:HD2	2.21	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	Interatomic distance (Å)	Clash overlap (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:NH2	2:K:21:LEU:C[2_554]	1.20	1.00
2:O:24:ARG:CZ	2:K:22:SER:N[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	2:K:24:ARG:NE[2_554]	1.89	0.31
2:O:81:GLN:CG	2:K:24:ARG:CZ[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
2:O:81:GLN:OE1	2:K:24:ARG:CZ[2_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	B	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	C	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	D	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	E	377/383 (98%)	356 (94%)	21 (6%)	21	29
1	F	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	G	377/383 (98%)	357 (95%)	20 (5%)	22	31
1	H	377/383 (98%)	356 (94%)	21 (6%)	21	29
2	I	99/104 (95%)	98 (99%)	1 (1%)	76	87
2	J	99/104 (95%)	98 (99%)	1 (1%)	76	87
2	K	99/104 (95%)	98 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	99/104 (95%)	98 (99%)	1 (1%)	76 87
2	M	99/104 (95%)	98 (99%)	1 (1%)	76 87
2	N	99/104 (95%)	98 (99%)	1 (1%)	76 87
2	O	99/104 (95%)	98 (99%)	1 (1%)	76 87
2	P	99/104 (95%)	98 (99%)	1 (1%)	76 87
All	All	3808/3896 (98%)	3638 (96%)	170 (4%)	27 39

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	D	476	-	15,17,17	2.22	6 (40%)	16,25,25	1.86	2 (12%)
3	XBP	B	476	-	15,17,17	2.22	5 (33%)	16,25,25	1.86	2 (12%)
3	XBP	H	476	-	15,17,17	2.21	6 (40%)	16,25,25	1.86	2 (12%)
3	XBP	F	476	1	15,17,17	2.22	6 (40%)	16,25,25	1.86	2 (12%)
3	XBP	C	476	-	15,17,17	2.21	6 (40%)	16,25,25	1.86	2 (12%)
3	XBP	A	476	-	15,17,17	2.21	6 (40%)	16,25,25	1.86	2 (12%)
3	XBP	G	476	1	15,17,17	2.21	6 (40%)	16,25,25	1.85	2 (12%)
3	XBP	E	476	-	15,17,17	2.22	6 (40%)	16,25,25	1.87	2 (12%)

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	D	476	-	-	6/20/20/20	-
3	XBP	B	476	-	-	6/20/20/20	-
3	XBP	H	476	-	-	6/20/20/20	-
3	XBP	F	476	1	-	6/20/20/20	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XBP	C	476	-	-	6/20/20/20	-
3	XBP	A	476	-	-	6/20/20/20	-
3	XBP	G	476	1	-	6/20/20/20	-
3	XBP	E	476	-	-	6/20/20/20	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	476	XBP	O1-C1	5.53	1.47	1.43
3	F	476	XBP	O1-C1	5.49	1.46	1.43
3	D	476	XBP	O1-C1	5.47	1.46	1.43
3	B	476	XBP	O1-C1	5.46	1.46	1.43
3	C	476	XBP	O1-C1	5.42	1.46	1.43
3	H	476	XBP	O1-C1	5.41	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	-3.55	1.48	1.60
3	B	476	XBP	P2-O5	-3.52	1.48	1.60
3	H	476	XBP	P2-O5	-3.51	1.48	1.60
3	D	476	XBP	P2-O5	-3.51	1.48	1.60
3	F	476	XBP	P2-O5	-3.51	1.48	1.60
3	A	476	XBP	P2-O5	-3.51	1.48	1.60
3	C	476	XBP	P2-O5	-3.50	1.49	1.60
3	E	476	XBP	P2-O5	-3.43	1.49	1.60
3	B	476	XBP	P1-O1	-2.72	1.51	1.60
3	D	476	XBP	P1-O1	-2.71	1.51	1.60
3	E	476	XBP	P1-O1	-2.71	1.51	1.60
3	C	476	XBP	P1-O1	-2.71	1.51	1.60
3	F	476	XBP	P1-O1	-2.70	1.51	1.60
3	A	476	XBP	P1-O1	-2.69	1.51	1.60
3	G	476	XBP	P1-O1	-2.69	1.51	1.60
3	H	476	XBP	P1-O1	-2.68	1.51	1.60
3	D	476	XBP	P1-O1P	2.68	1.59	1.50
3	G	476	XBP	P1-O1P	2.68	1.59	1.50
3	F	476	XBP	P1-O1P	2.67	1.59	1.50
3	C	476	XBP	P1-O1P	2.67	1.59	1.50
3	B	476	XBP	P1-O1P	2.66	1.59	1.50
3	A	476	XBP	P1-O1P	2.66	1.59	1.50
3	H	476	XBP	P1-O1P	2.65	1.59	1.50
3	E	476	XBP	P1-O1P	2.61	1.59	1.50
3	B	476	XBP	P2-O4P	2.24	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	476	XBP	P2-O4P	2.24	1.57	1.50
3	F	476	XBP	P2-O4P	2.23	1.57	1.50
3	C	476	XBP	P2-O4P	2.23	1.57	1.50
3	A	476	XBP	P2-O4P	2.22	1.57	1.50
3	G	476	XBP	P2-O4P	2.22	1.57	1.50
3	D	476	XBP	P2-O4P	2.21	1.57	1.50
3	E	476	XBP	P2-O4P	2.19	1.57	1.50
3	C	476	XBP	P2-O6P	2.03	1.62	1.54
3	D	476	XBP	P2-O6P	2.03	1.62	1.54
3	G	476	XBP	P2-O6P	2.02	1.62	1.54
3	H	476	XBP	P2-O6P	2.02	1.62	1.54
3	F	476	XBP	P2-O6P	2.02	1.62	1.54
3	A	476	XBP	P2-O6P	2.02	1.62	1.54
3	E	476	XBP	P2-O6P	2.01	1.62	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	476	XBP	O5-C5-C4	4.93	122.52	109.36
3	B	476	XBP	O5-C5-C4	4.88	122.40	109.36
3	A	476	XBP	O5-C5-C4	4.88	122.39	109.36
3	F	476	XBP	O5-C5-C4	4.88	122.39	109.36
3	D	476	XBP	O5-C5-C4	4.88	122.39	109.36
3	C	476	XBP	O5-C5-C4	4.88	122.38	109.36
3	H	476	XBP	O5-C5-C4	4.88	122.38	109.36
3	G	476	XBP	O5-C5-C4	4.85	122.30	109.36
3	E	476	XBP	P2-O5-C5	3.83	128.86	118.30
3	C	476	XBP	P2-O5-C5	3.82	128.82	118.30
3	H	476	XBP	P2-O5-C5	3.82	128.81	118.30
3	F	476	XBP	P2-O5-C5	3.81	128.80	118.30
3	D	476	XBP	P2-O5-C5	3.81	128.79	118.30
3	A	476	XBP	P2-O5-C5	3.81	128.78	118.30
3	B	476	XBP	P2-O5-C5	3.80	128.77	118.30
3	G	476	XBP	P2-O5-C5	3.78	128.72	118.30

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	476	XBP	O2-C2-C3-O3
3	D	476	XBP	C5-O5-P2-O4P
3	D	476	XBP	C5-O5-P2-O5P

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Mol	Chain	Res	Type	Atoms
3	B	476	XBP	O2-C2-C3-O3
3	B	476	XBP	C5-O5-P2-O4P
3	B	476	XBP	C5-O5-P2-O5P
3	H	476	XBP	O2-C2-C3-O3
3	H	476	XBP	C5-O5-P2-O4P
3	H	476	XBP	C5-O5-P2-O5P
3	F	476	XBP	O2-C2-C3-O3
3	F	476	XBP	C5-O5-P2-O4P
3	F	476	XBP	C5-O5-P2-O5P
3	C	476	XBP	O2-C2-C3-O3
3	C	476	XBP	C5-O5-P2-O4P
3	C	476	XBP	C5-O5-P2-O5P
3	A	476	XBP	O2-C2-C3-O3
3	A	476	XBP	C5-O5-P2-O4P
3	A	476	XBP	C5-O5-P2-O5P
3	G	476	XBP	O2-C2-C3-O3
3	G	476	XBP	C5-O5-P2-O4P
3	G	476	XBP	C5-O5-P2-O5P
3	E	476	XBP	O2-C2-C3-O3
3	E	476	XBP	C5-O5-P2-O4P
3	E	476	XBP	C5-O5-P2-O5P
3	D	476	XBP	C4-C5-O5-P2
3	B	476	XBP	C4-C5-O5-P2
3	H	476	XBP	C4-C5-O5-P2
3	F	476	XBP	C4-C5-O5-P2
3	E	476	XBP	C4-C5-O5-P2
3	C	476	XBP	C4-C5-O5-P2
3	A	476	XBP	C4-C5-O5-P2
3	G	476	XBP	C4-C5-O5-P2
3	D	476	XBP	C1-C2-C3-C4
3	B	476	XBP	C1-C2-C3-C4
3	H	476	XBP	C1-C2-C3-C4
3	F	476	XBP	C1-C2-C3-C4
3	C	476	XBP	C1-C2-C3-C4
3	A	476	XBP	C1-C2-C3-C4
3	G	476	XBP	C1-C2-C3-C4
3	E	476	XBP	C1-C2-C3-C4
3	D	476	XBP	C5-O5-P2-O6P
3	B	476	XBP	C5-O5-P2-O6P
3	H	476	XBP	C5-O5-P2-O6P
3	F	476	XBP	C5-O5-P2-O6P
3	C	476	XBP	C5-O5-P2-O6P

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Mol	Chain	Res	Type	Atoms
3	A	476	XBP	C5-O5-P2-O6P
3	G	476	XBP	C5-O5-P2-O6P
3	E	476	XBP	C5-O5-P2-O6P

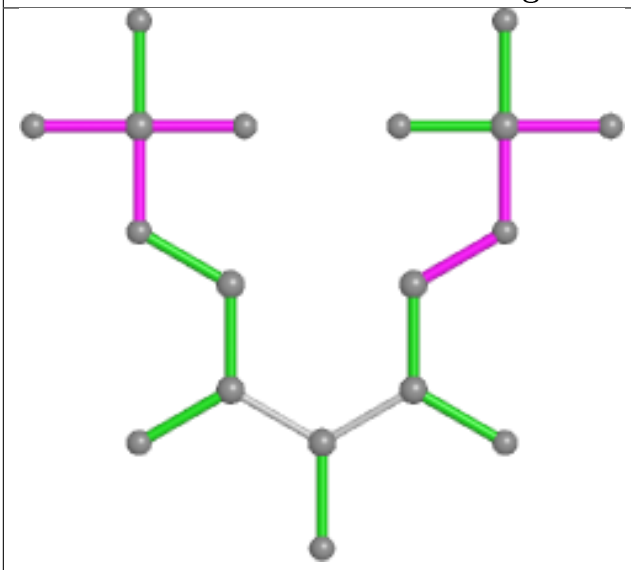
There are no ring outliers.

8 monomers are involved in 14 short contacts:

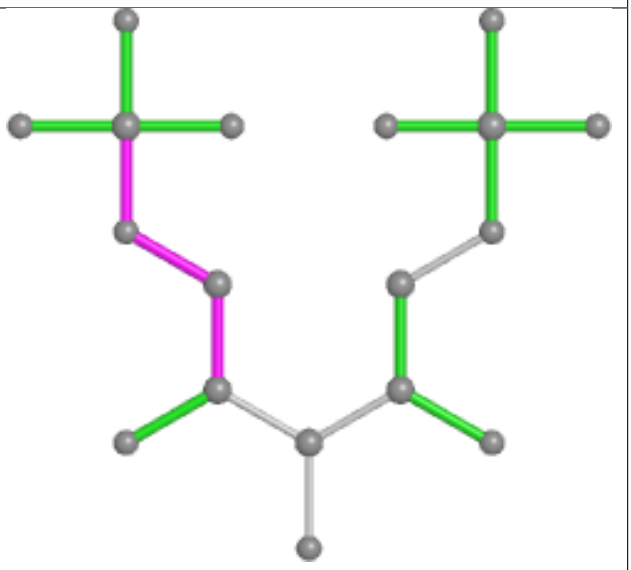
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	476	XBP	2	0
3	B	476	XBP	2	0
3	H	476	XBP	2	0
3	F	476	XBP	1	0
3	C	476	XBP	2	0
3	A	476	XBP	2	0
3	G	476	XBP	1	0
3	E	476	XBP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

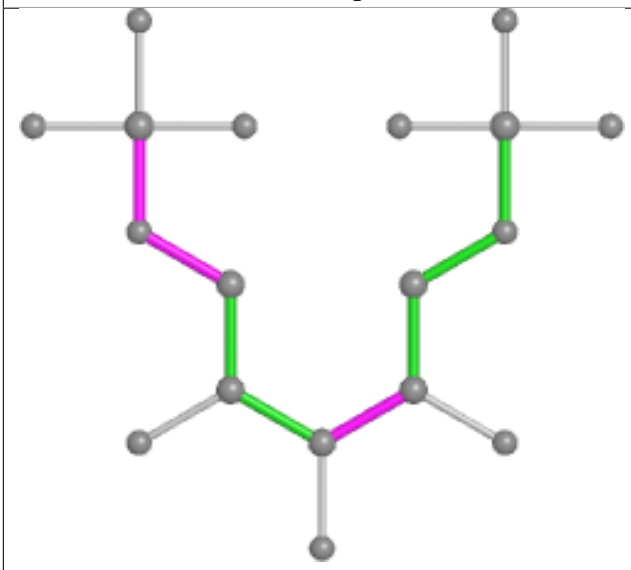
Ligand XBP D 476



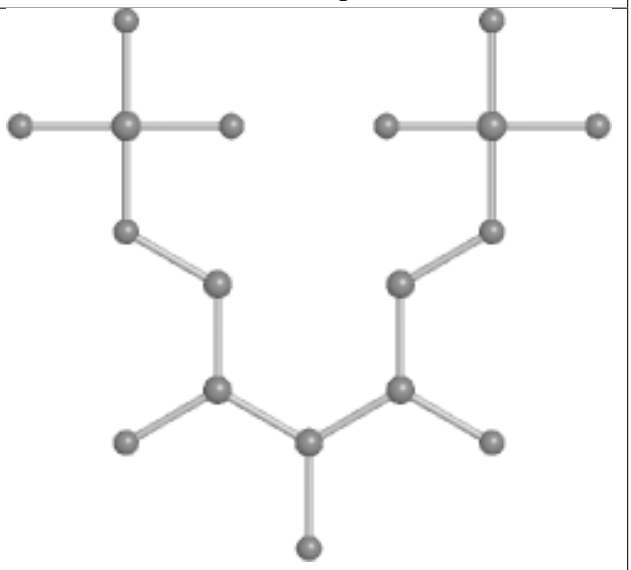
Bond lengths



Bond angles

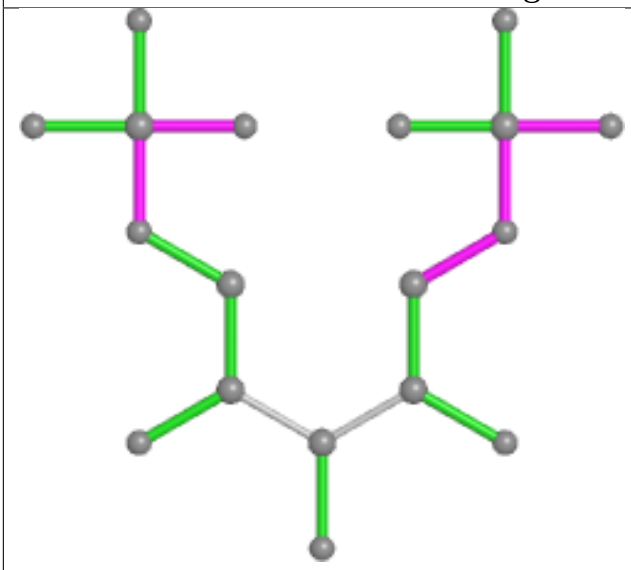


Torsions

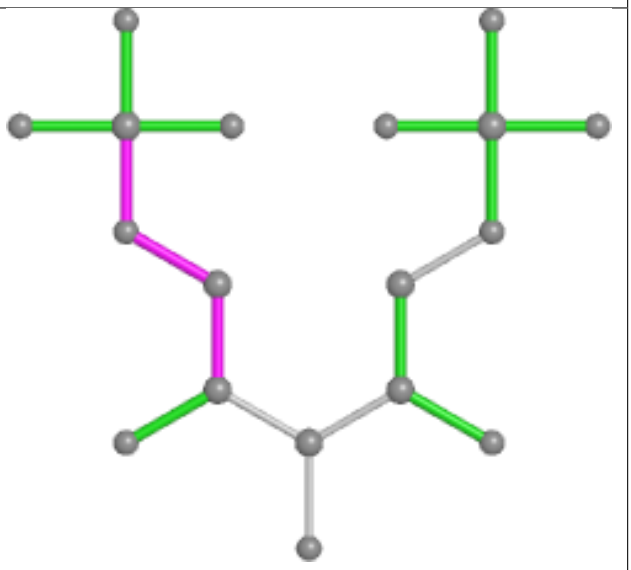


Rings

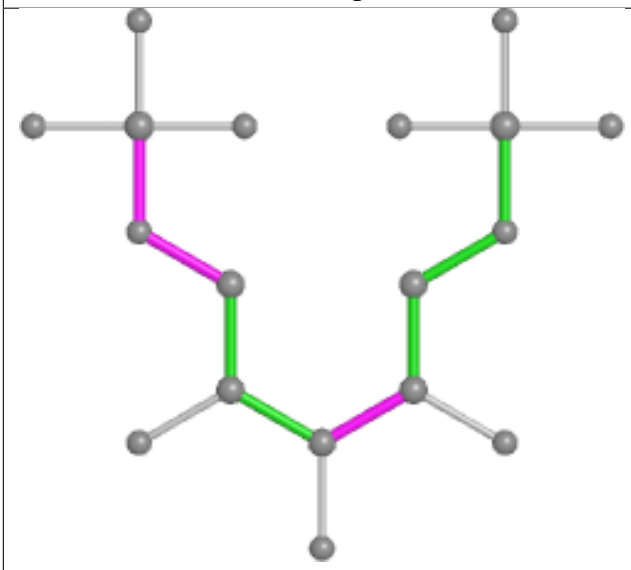
Ligand XBP B 476



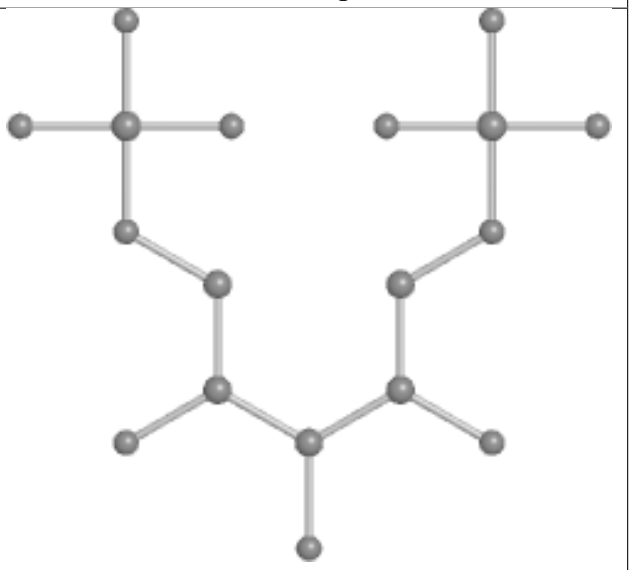
Bond lengths



Bond angles

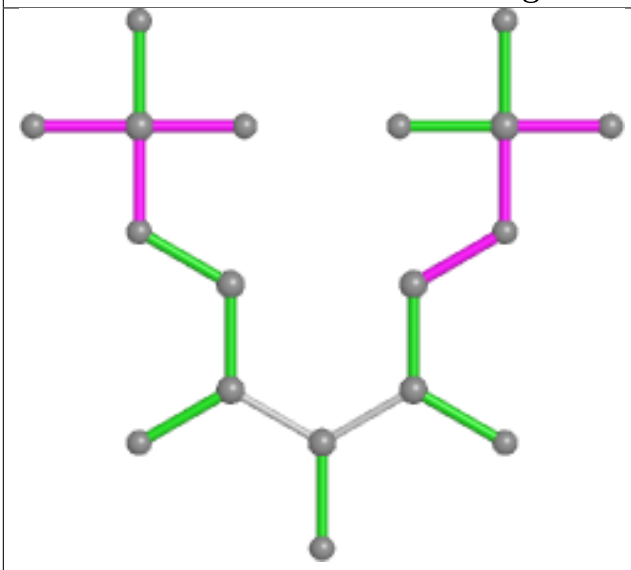


Torsions

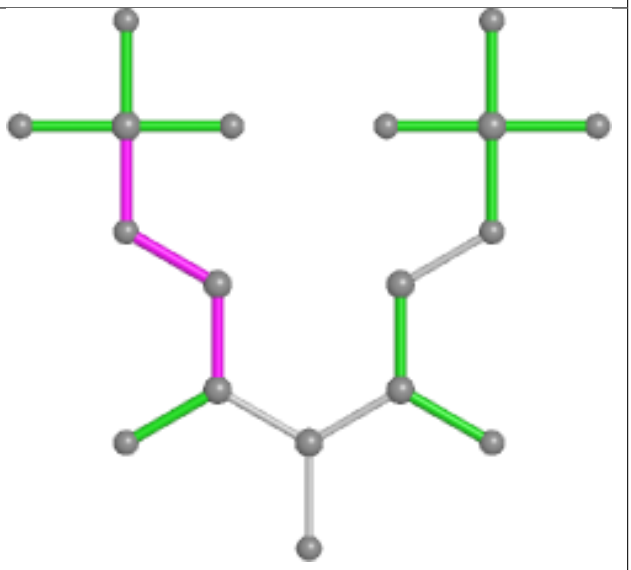


Rings

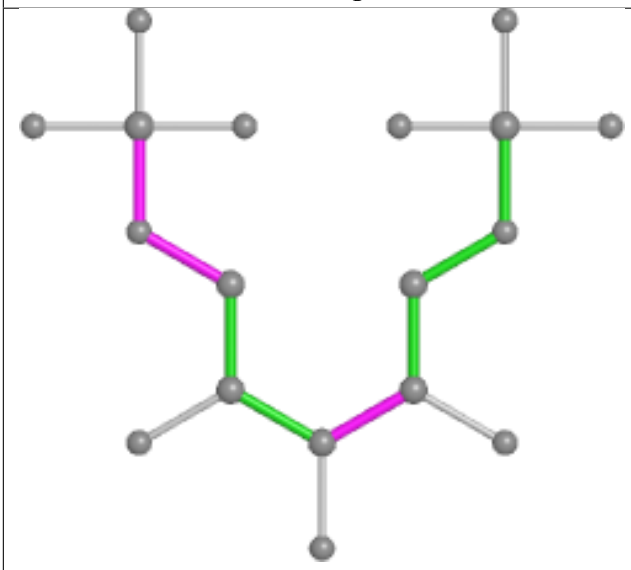
Ligand XBP H 476



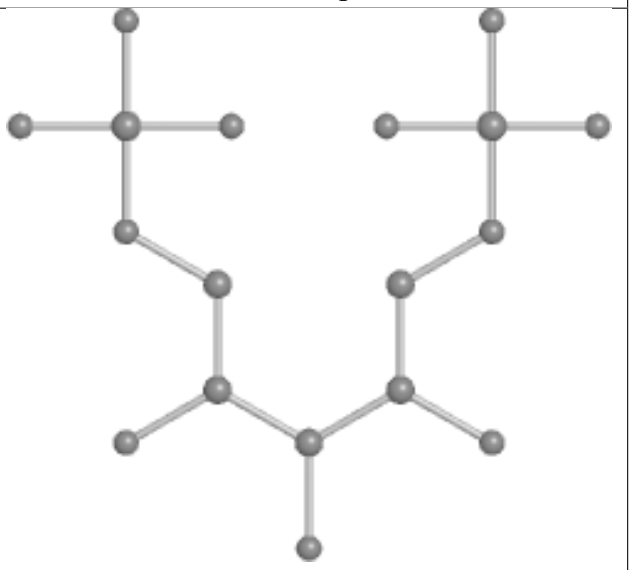
Bond lengths



Bond angles

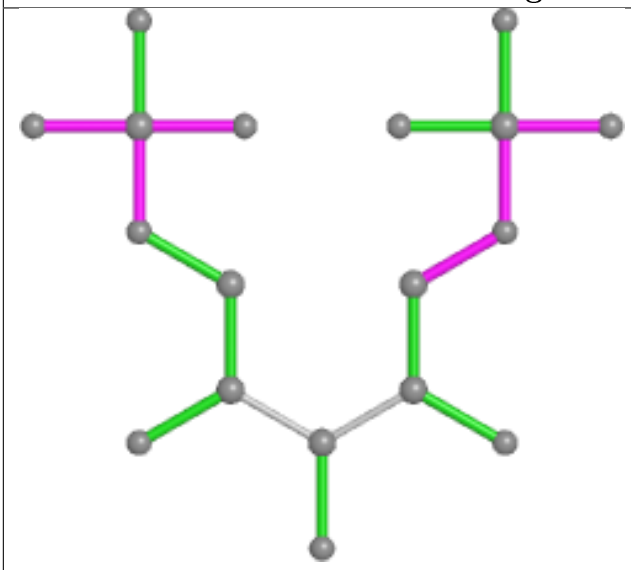


Torsions

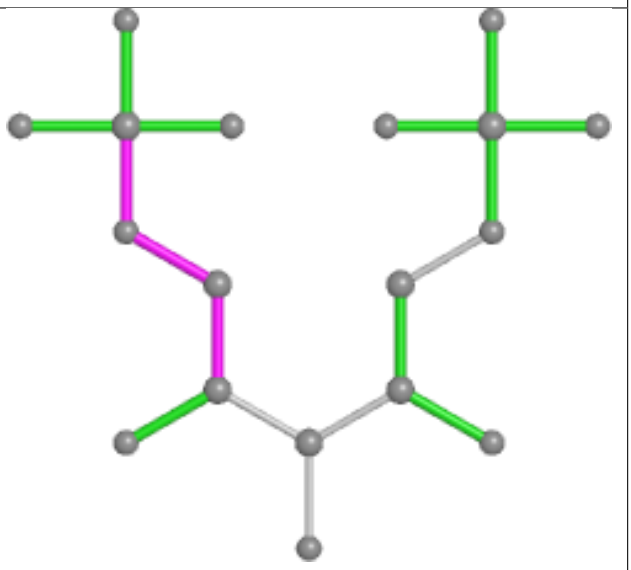


Rings

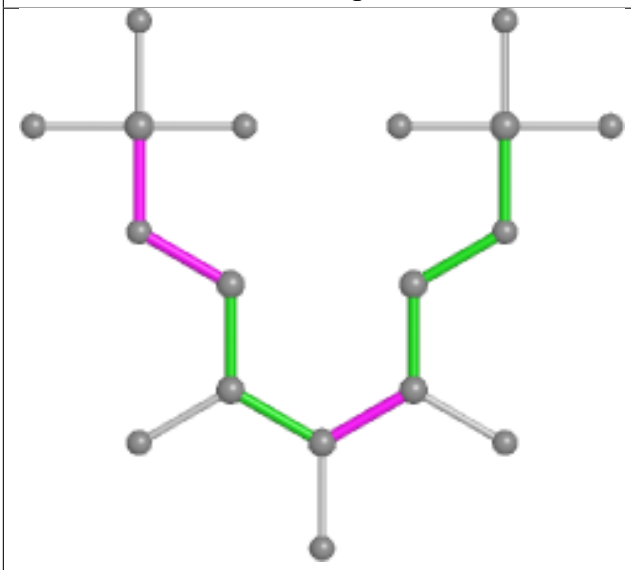
Ligand XBP F 476



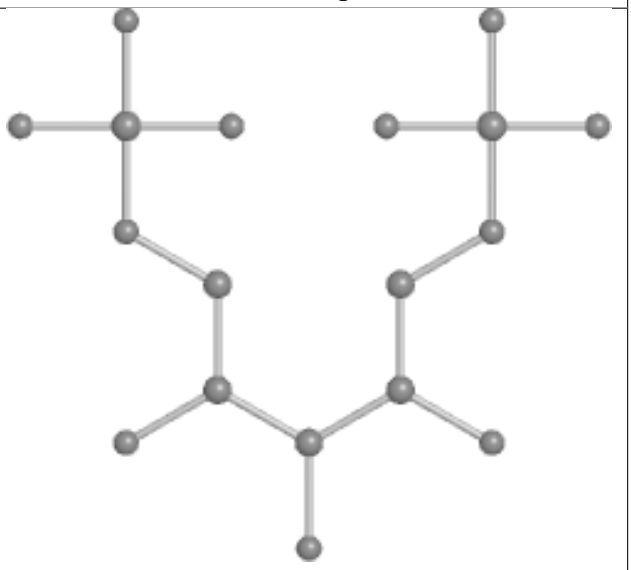
Bond lengths



Bond angles

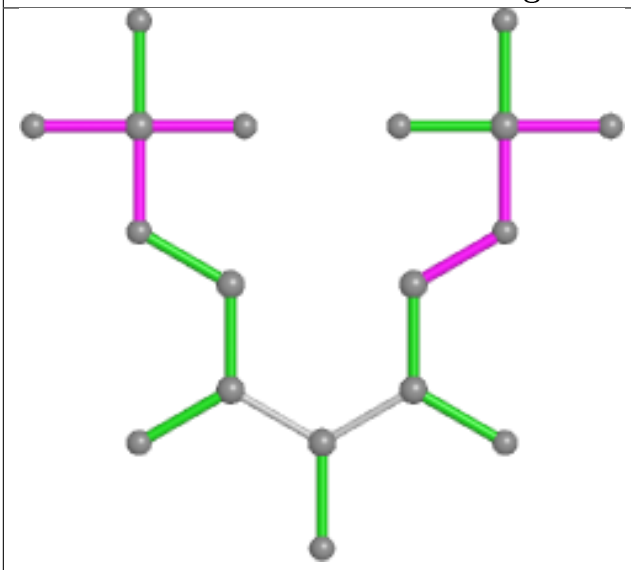


Torsions

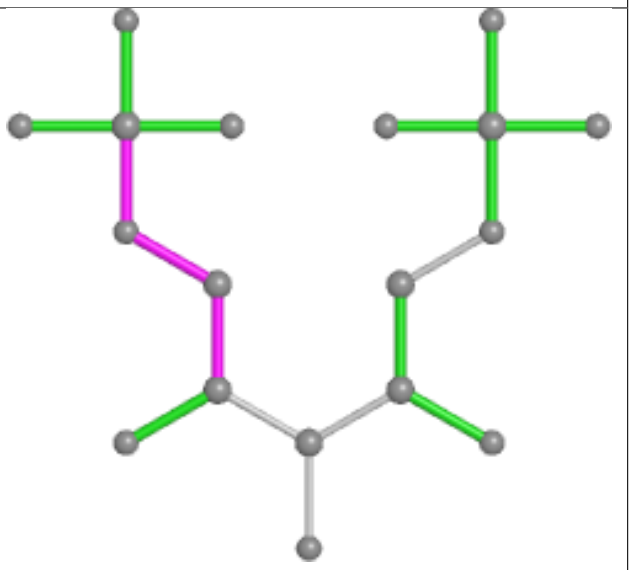


Rings

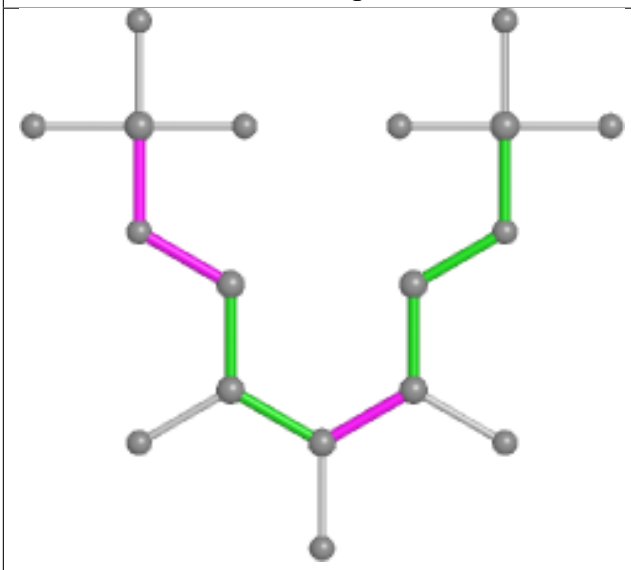
Ligand XBP C 476



Bond lengths



Bond angles



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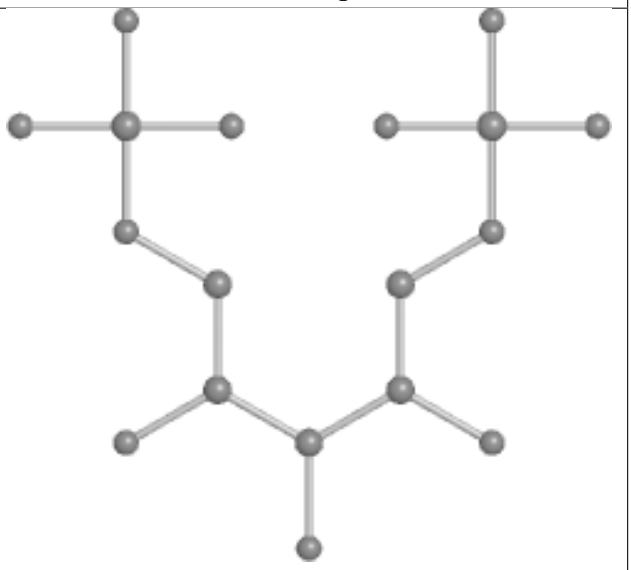
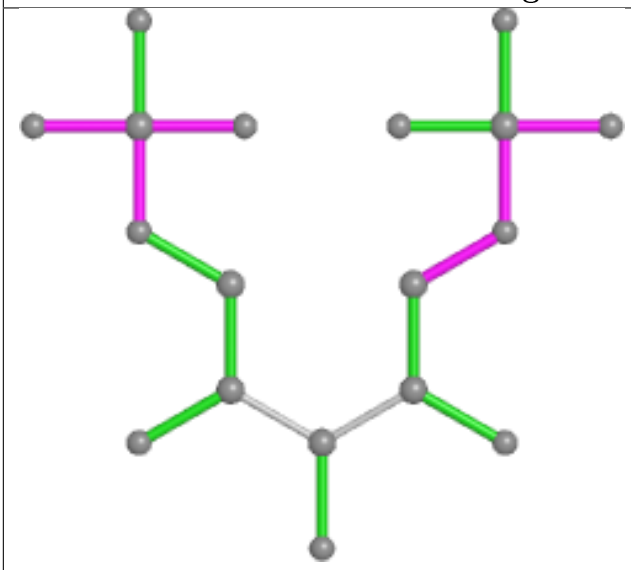


Rings

Ligand XBP A 476



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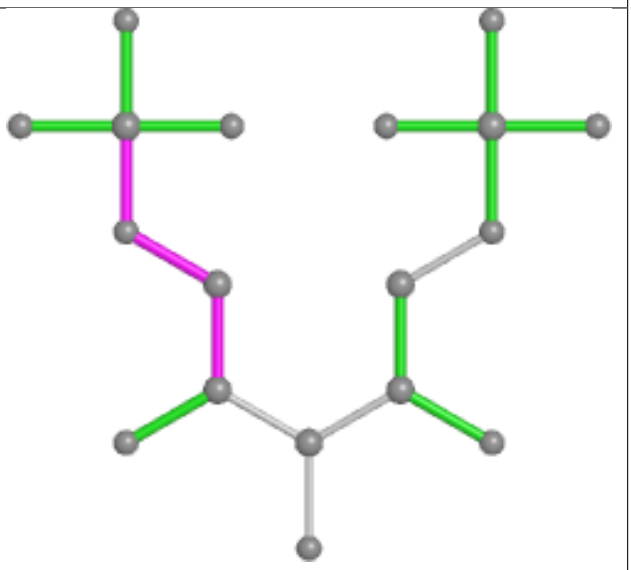
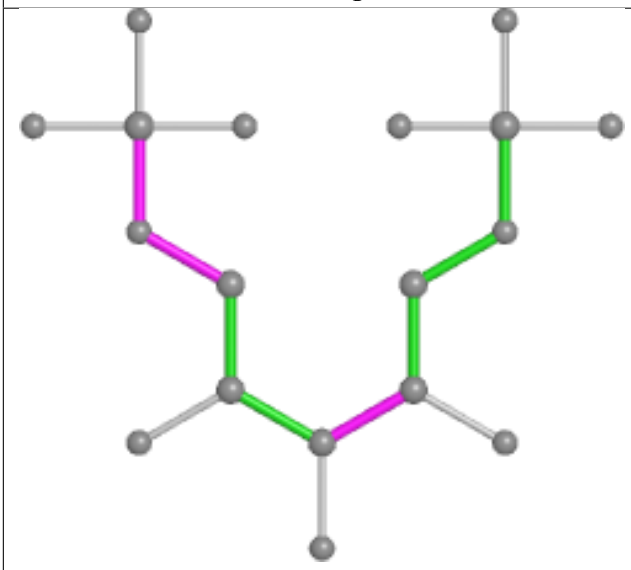


Bond angles



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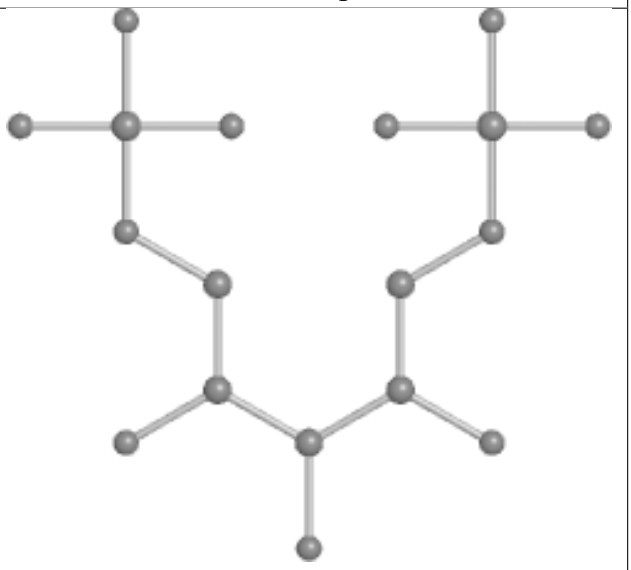
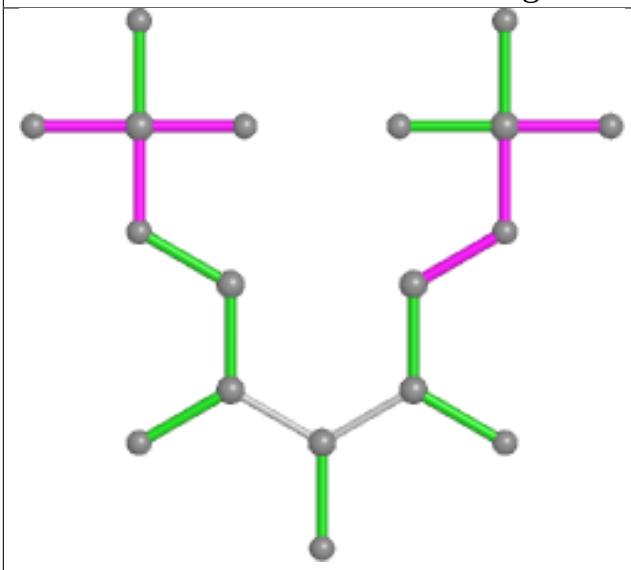
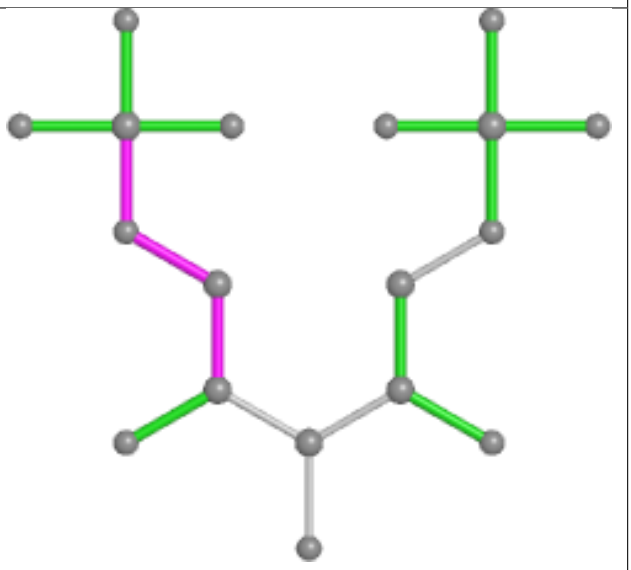


Rings

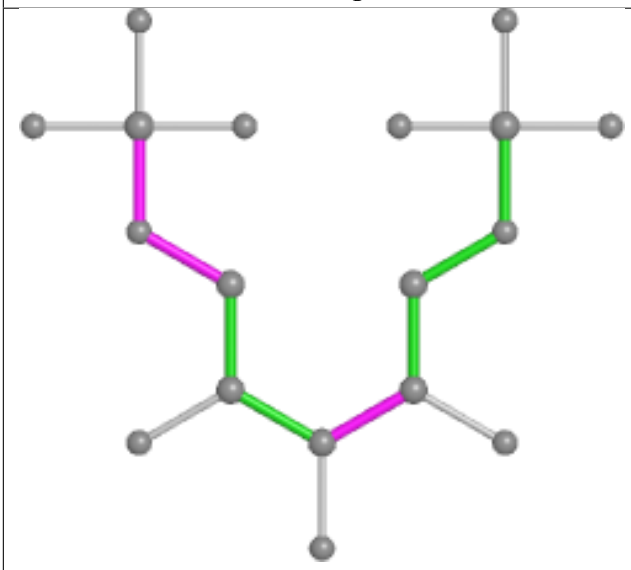
Ligand XBP G 476



Bond lengths



Bond angles



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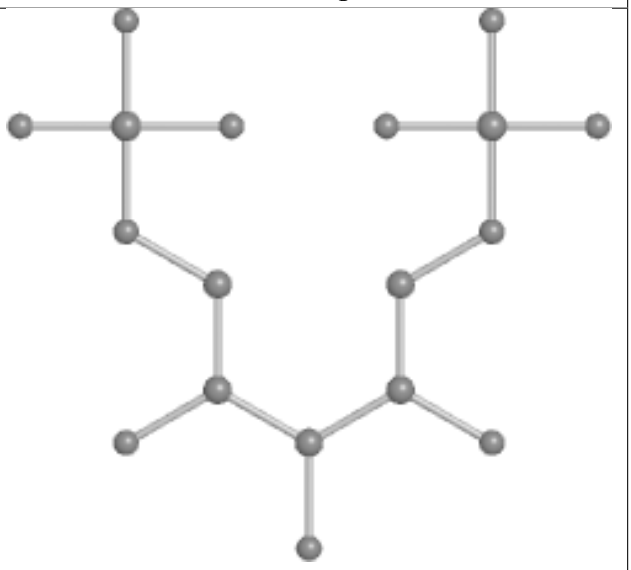
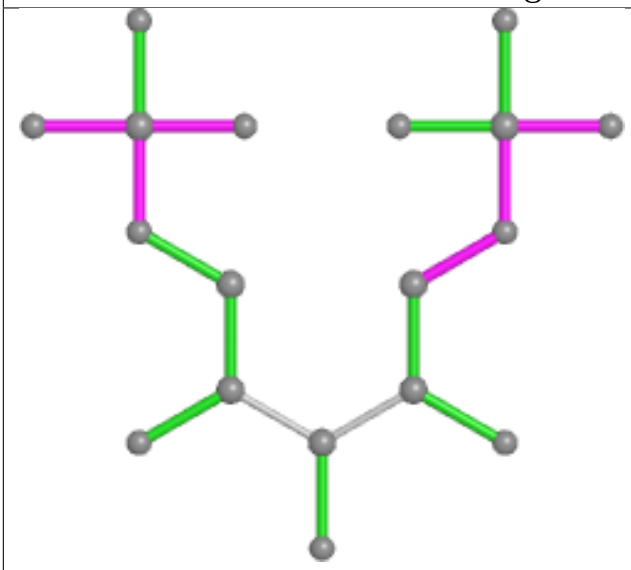


Rings

Ligand XBP E 476



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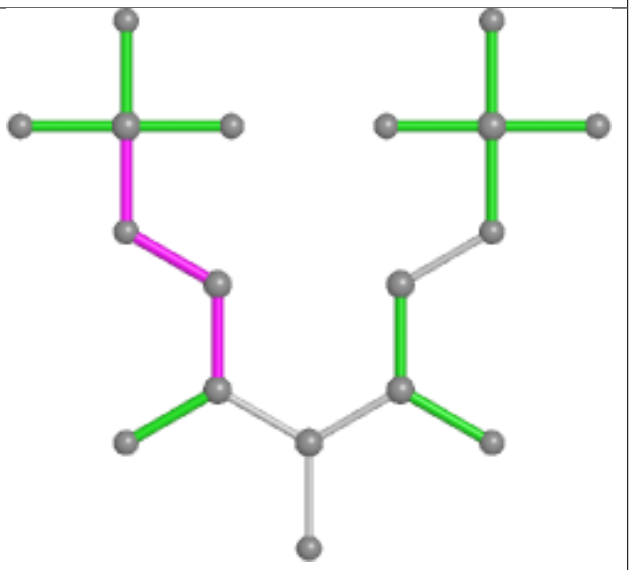

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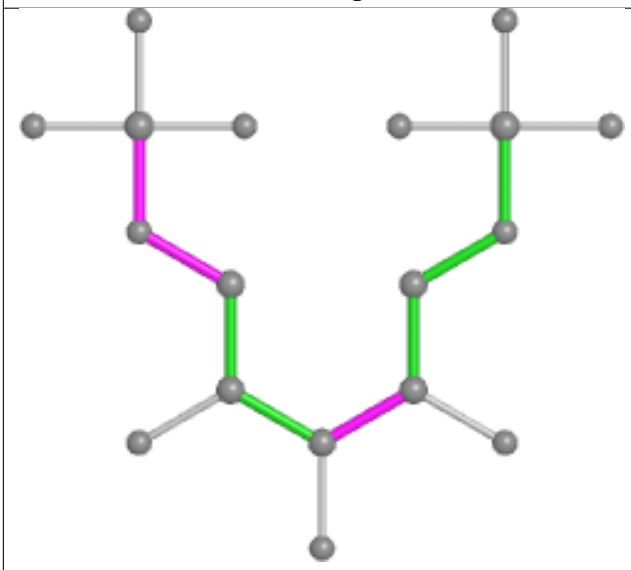
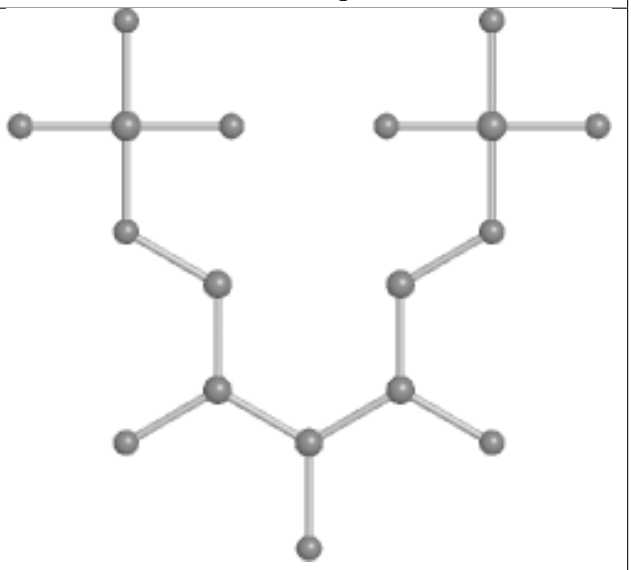


Torsions



Rings

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.