



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:24 AM UTC

PDB ID : 2HCK / pdb_00002hck
Title : SRC FAMILY KINASE HCK-QUERCETIN COMPLEX
Authors : Sicheri, F.; Moarefi, I.; Kuriyan, J.
Deposited on : 1997-02-25
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

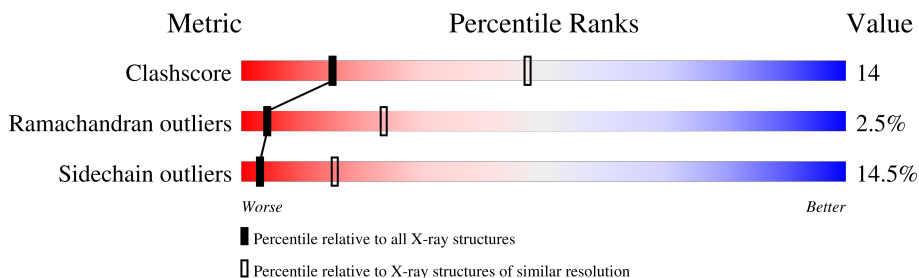
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	438	50% 35% 13% .
1	B	438	45% 41% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	QUE	B	532	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8556 atoms, of which 1536 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 HEMATOPOETIC CELL KINASE HCK.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	P	S	0	0	0
			4253	2232	768	585	647	1	20			
1	B	438	Total	C	H	N	O	P	S	0	0	0
			4253	2232	768	585	647	1	20			

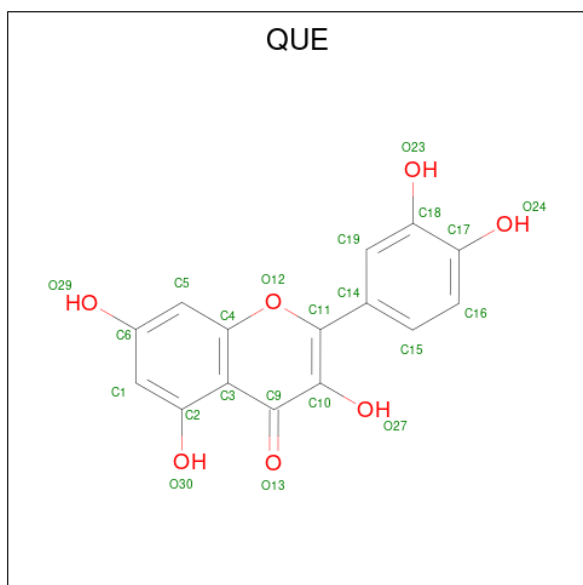
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	ASP	deletion	UNP P08631
A	?	-	ASN	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	?	-	TYR	deletion	UNP P08631
A	?	-	THR	deletion	UNP P08631
A	?	-	ALA	deletion	UNP P08631
A	?	-	ARG	deletion	UNP P08631
A	?	-	GLU	deletion	UNP P08631
A	527	PTR	TYR	modified residue	UNP P08631
B	?	-	ILE	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	ASP	deletion	UNP P08631
B	?	-	ASN	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	?	-	TYR	deletion	UNP P08631
B	?	-	THR	deletion	UNP P08631
B	?	-	ALA	deletion	UNP P08631
B	?	-	ARG	deletion	UNP P08631
B	?	-	GLU	deletion	UNP P08631
B	527	PTR	TYR	modified residue	UNP P08631

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: C₁₅H₁₀O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 22 15 7	0	0
3	B	1	Total C O 22 15 7	0	0

- Molecule 4 is water.

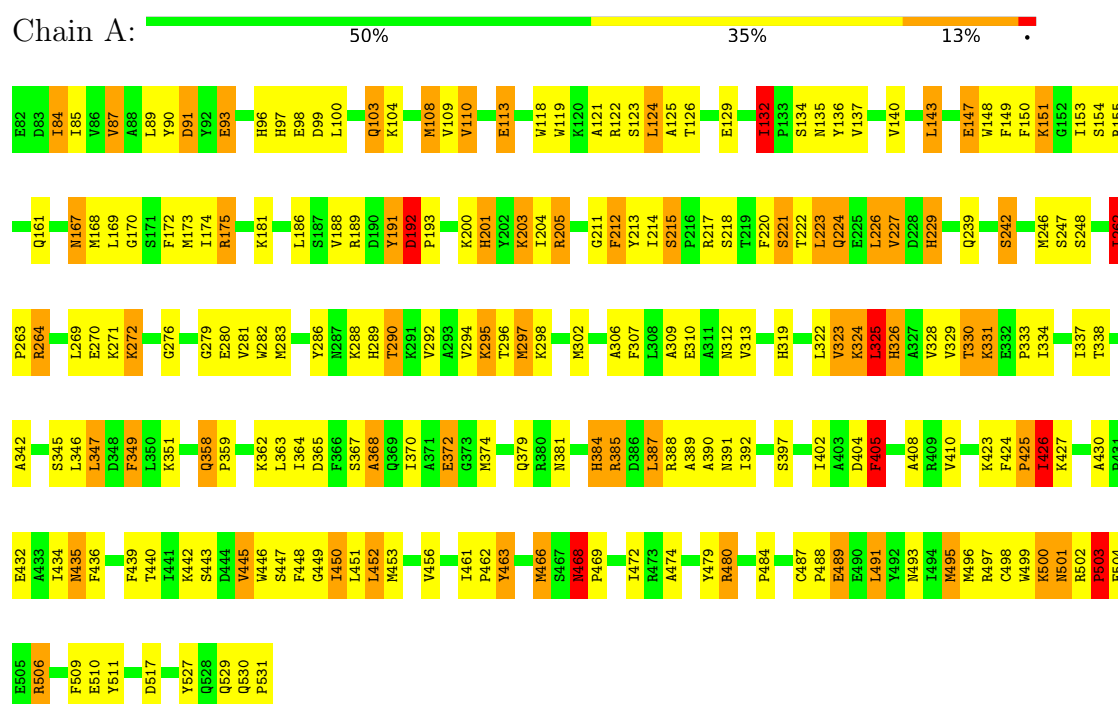
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0

3 Residue-property plots

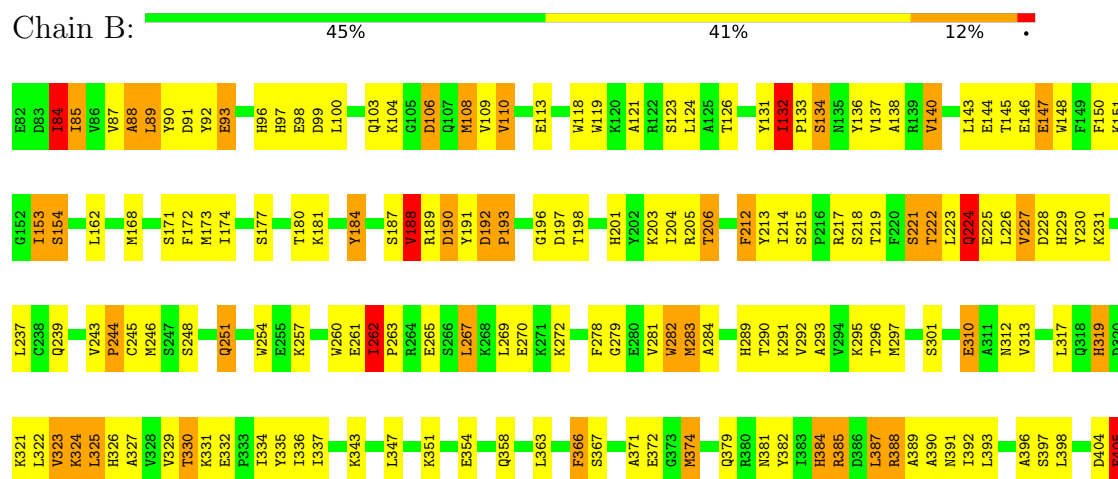
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

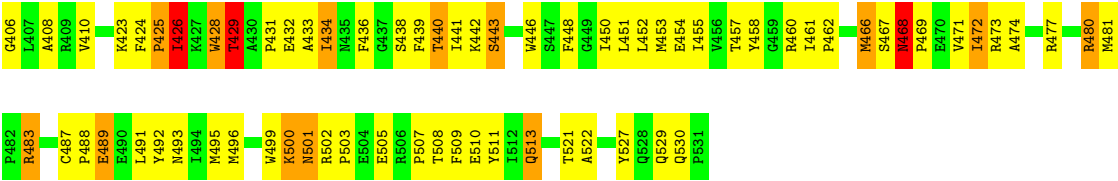
Note EDS was not executed.

• Molecule 1: HEMATOPOETIC CELL KINASE HCK



• Molecule 1: HEMATOPOETIC CELL KINASE HCK





4 Data and refinement statistics

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	73.50Å 93.30Å 176.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.1 (18.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.228 , 0.311	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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: CA, QUE, PTR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.20	16/3552 (0.5%)	2.04	122/4799 (2.5%)
1	B	1.20	12/3552 (0.3%)	2.12	151/4799 (3.1%)
All	All	1.20	28/7104 (0.4%)	2.08	273/9598 (2.8%)

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	1
1	B	0	3
All	All	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	ILE	CA-CB	8.62	1.61	1.54
1	B	229	HIS	CD2-NE2	-7.37	1.29	1.37
1	B	97	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	97	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	364	ILE	CA-CB	6.94	1.63	1.54
1	A	96	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	384	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	319	HIS	CD2-NE2	-6.74	1.30	1.37
1	B	326	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	319	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	384	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	110	VAL	CA-CB	6.32	1.62	1.54
1	A	201	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	319	HIS	CG-ND1	-5.89	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	ILE	CA-CB	5.80	1.61	1.54
1	A	326	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	370	ILE	CA-CB	-5.77	1.47	1.54
1	A	506	ARG	CA-CB	-5.75	1.45	1.53
1	B	201	HIS	CD2-NE2	-5.69	1.31	1.37
1	B	96	HIS	CD2-NE2	-5.68	1.31	1.37
1	A	511	TYR	CA-CB	5.58	1.61	1.53
1	B	229	HIS	CG-ND1	-5.49	1.32	1.38
1	A	289	HIS	CD2-NE2	-5.39	1.31	1.37
1	B	289	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	229	HIS	CD2-NE2	-5.37	1.31	1.37
1	B	374	MET	CA-CB	-5.07	1.45	1.53
1	B	201	HIS	CG-ND1	-5.06	1.32	1.38
1	A	384	HIS	CG-ND1	-5.05	1.32	1.38

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	PHE	CA-CB-CG	10.78	124.58	113.80
1	A	276	GLY	N-CA-C	-9.92	98.98	112.57
1	A	368	ALA	N-CA-C	-9.38	101.04	111.07
1	A	135	ASN	CA-CB-CG	9.37	121.97	112.60
1	A	323	VAL	N-CA-CB	-9.36	101.79	111.90
1	B	509	PHE	CA-CB-CG	-9.30	104.50	113.80
1	B	97	HIS	N-CA-C	9.24	122.20	111.11
1	B	379	GLN	OE1-CD-NE2	-9.17	113.43	122.60
1	A	425	PRO	N-CA-C	9.11	131.24	112.47
1	A	229	HIS	CA-CB-CG	8.97	122.77	113.80
1	A	342	ALA	N-CA-C	8.87	122.07	111.33
1	B	262	ILE	CA-C-O	8.77	125.34	119.38
1	B	289	HIS	CA-CB-CG	8.47	122.27	113.80
1	A	262	ILE	CA-C-O	8.46	124.76	119.51
1	A	226	LEU	N-CA-C	-8.26	102.23	111.07
1	B	530	GLN	N-CA-C	8.23	121.39	109.71
1	B	367	SER	CA-CB-OG	-8.22	94.67	111.10
1	B	326	HIS	N-CA-C	8.21	123.84	112.93
1	B	391	ASN	OD1-CG-ND2	-8.21	114.39	122.60
1	B	405	PHE	CA-CB-CG	8.16	121.96	113.80
1	A	97	HIS	N-CA-C	8.15	120.96	111.02
1	B	197	ASP	CA-CB-CG	8.10	120.70	112.60
1	A	149	PHE	CA-CB-CG	-8.08	105.72	113.80
1	A	212	PHE	CA-CB-CG	8.08	121.88	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	MET	CG-SD-CE	-8.04	83.22	100.90
1	B	404	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	270	GLU	N-CA-C	7.85	122.12	112.23
1	B	468	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	391	ASN	CB-CG-ND2	7.70	127.94	116.40
1	B	131	TYR	N-CA-C	7.64	122.47	110.32
1	A	424	PHE	CA-C-N	7.62	129.37	119.84
1	A	424	PHE	C-N-CA	7.62	129.37	119.84
1	B	501	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	468	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	B	384	HIS	CB-CG-CD2	-7.48	121.48	131.20
1	B	374	MET	CA-CB-CG	-7.30	99.50	114.10
1	B	184	TYR	O-C-N	-7.26	113.75	123.19
1	B	443	SER	N-CA-C	-7.23	103.33	111.07
1	A	326	HIS	N-CA-C	7.23	122.54	112.93
1	A	493	ASN	CB-CG-ND2	7.21	127.22	116.40
1	B	462	PRO	N-CA-C	7.19	122.10	111.03
1	A	132	ILE	N-CA-CB	-7.05	101.33	111.21
1	B	99	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	93	GLU	N-CA-C	-7.00	95.69	107.80
1	A	423	LYS	N-CA-C	-6.98	102.35	111.71
1	B	147	GLU	N-CA-C	6.98	125.66	110.80
1	B	146	GLU	CB-CG-CD	6.97	124.45	112.60
1	A	205	ARG	CB-CG-CD	6.96	127.31	111.30
1	B	426	ILE	N-CA-C	6.95	123.79	109.34
1	B	366	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	272	LYS	N-CA-C	-6.92	99.42	109.59
1	A	148	TRP	CG-CD2-CE3	6.92	140.82	133.90
1	A	201	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	A	151	LYS	N-CA-C	6.90	125.49	110.80
1	B	511	TYR	N-CA-C	-6.88	103.86	111.36
1	B	187	SER	CA-C-O	-6.86	113.41	121.16
1	B	143	LEU	N-CA-C	6.84	125.38	110.80
1	B	325	LEU	O-C-N	-6.84	114.51	122.93
1	B	192	ASP	CA-C-N	6.82	127.38	119.47
1	B	192	ASP	C-N-CA	6.82	127.38	119.47
1	A	391	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	405	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	439	PHE	CA-CB-CG	6.78	120.58	113.80
1	B	384	HIS	CB-CG-ND1	6.78	132.86	122.70
1	B	103	GLN	OE1-CD-NE2	-6.75	115.85	122.60
1	A	517	ASP	CA-CB-CG	6.75	119.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	SER	N-CA-C	6.73	121.09	112.34
1	A	167	ASN	N-CA-C	-6.66	101.94	110.53
1	B	239	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	392	ILE	N-CA-C	-6.66	98.79	108.11
1	A	365	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	381	ASN	CA-CB-CG	6.64	119.24	112.60
1	B	312	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	B	425	PRO	N-CA-C	6.63	126.13	112.47
1	B	84	ILE	N-CA-C	6.54	117.85	107.98
1	B	529	GLN	O-C-N	6.54	130.73	123.01
1	B	106	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	529	GLN	CB-CG-CD	6.53	123.70	112.60
1	A	87	VAL	N-CA-C	6.51	118.09	108.45
1	A	424	PHE	CA-CB-CG	6.50	120.30	113.80
1	B	239	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	A	192	ASP	CA-C-N	6.45	126.95	119.47
1	A	192	ASP	C-N-CA	6.45	126.95	119.47
1	B	529	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	B	324	LYS	CG-CD-CE	6.38	125.96	111.30
1	A	384	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	181	LYS	N-CA-C	6.36	118.76	110.43
1	B	489	GLU	CB-CG-CD	6.36	123.41	112.60
1	A	468	ASN	N-CA-C	6.35	123.84	109.81
1	A	215	SER	CA-C-O	-6.35	114.10	120.64
1	A	91	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	468	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	491	LEU	N-CA-C	-6.32	103.69	111.40
1	B	513	GLN	N-CA-C	-6.32	104.31	111.07
1	A	204	ILE	N-CA-C	-6.29	99.30	108.11
1	A	445	VAL	CA-C-O	-6.25	114.55	121.17
1	B	270	GLU	O-C-N	-6.24	113.55	122.41
1	A	372	GLU	CB-CG-CD	6.22	123.18	112.60
1	B	410	VAL	O-C-N	-6.20	117.39	122.97
1	A	426	ILE	N-CA-C	6.20	122.24	109.34
1	A	113	GLU	CA-CB-CG	-6.20	101.71	114.10
1	B	330	THR	N-CA-C	6.18	118.99	111.82
1	B	505	GLU	CB-CG-CD	6.17	123.09	112.60
1	A	370	ILE	N-CA-C	-6.17	104.49	110.72
1	A	203	LYS	CG-CD-CE	-6.17	97.12	111.30
1	A	451	LEU	N-CA-C	-6.16	104.65	111.36
1	B	468	ASN	CA-C-O	-6.14	111.74	120.16
1	B	381	ASN	OD1-CG-ND2	-6.14	116.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ARG	CB-CG-CD	-6.12	97.21	111.30
1	A	96	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	A	410	VAL	N-CA-C	6.11	116.81	107.77
1	A	389	ALA	CA-C-O	6.11	127.22	120.63
1	B	343	LYS	N-CA-C	6.10	119.43	112.97
1	A	99	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	92	TYR	N-CA-C	-6.09	100.08	109.52
1	B	221	SER	CA-C-O	6.08	126.66	119.06
1	A	349	PHE	CA-CB-CG	-6.05	107.75	113.80
1	A	161	GLN	N-CA-C	6.04	117.87	111.28
1	B	501	ASN	CB-CG-ND2	6.03	125.44	116.40
1	A	404	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	206	THR	O-C-N	-6.02	115.18	123.12
1	A	297	MET	N-CA-C	6.01	118.54	108.02
1	A	172	PHE	N-CA-C	6.01	116.02	108.45
1	B	88	ALA	N-CA-C	6.01	117.80	109.15
1	B	221	SER	N-CA-C	-6.00	106.60	114.04
1	B	436	PHE	CA-CB-CG	5.99	119.79	113.80
1	B	118	TRP	CG-CD2-CE3	5.98	139.88	133.90
1	A	506	ARG	N-CA-C	-5.98	102.06	110.31
1	B	310	GLU	CB-CG-CD	5.97	122.75	112.60
1	B	379	GLN	CB-CG-CD	5.94	122.70	112.60
1	B	374	MET	N-CA-CB	-5.93	101.16	110.06
1	B	144	GLU	CB-CG-CD	5.92	122.66	112.60
1	B	184	TYR	N-CA-C	5.92	119.19	109.72
1	A	289	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	298	LYS	N-CA-C	5.89	116.82	109.57
1	B	332	GLU	O-C-N	-5.88	114.56	121.32
1	A	170	GLY	N-CA-C	-5.87	107.71	114.69
1	B	239	GLN	N-CA-C	5.85	118.07	109.24
1	A	325	LEU	N-CA-C	-5.84	100.47	109.76
1	A	362	LYS	N-CA-C	-5.84	104.51	111.69
1	B	97	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	B	206	THR	N-CA-C	5.83	118.23	108.02
1	B	190	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	96	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	B	201	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	A	93	GLU	CB-CG-CD	5.80	122.46	112.60
1	A	510	GLU	CB-CG-CD	5.78	122.43	112.60
1	A	148	TRP	CB-CG-CD1	-5.78	118.23	126.90
1	B	193	PRO	N-CA-C	5.78	122.18	113.81
1	B	265	GLU	CB-CG-CD	5.77	122.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	THR	N-CA-C	5.77	117.24	111.07
1	A	501	ASN	N-CA-C	5.77	119.42	112.38
1	B	262	ILE	CA-C-N	5.75	127.03	119.84
1	B	262	ILE	C-N-CA	5.75	127.03	119.84
1	A	379	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	A	218	SER	O-C-N	-5.73	117.22	123.52
1	A	502	ARG	CA-C-N	5.73	127.00	119.84
1	A	502	ARG	C-N-CA	5.73	127.00	119.84
1	B	502	ARG	CA-C-N	5.70	125.81	119.32
1	B	502	ARG	C-N-CA	5.70	125.81	119.32
1	A	239	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	B	393	LEU	CA-C-O	-5.68	114.81	121.46
1	B	468	ASN	O-C-N	-5.66	114.81	121.32
1	B	323	VAL	N-CA-CB	-5.63	104.64	110.95
1	B	384	HIS	N-CA-C	-5.63	95.33	107.49
1	A	279	GLY	O-C-N	5.63	129.94	123.58
1	A	435	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	224	GLN	CB-CG-CD	5.62	122.15	112.60
1	B	84	ILE	O-C-N	-5.61	116.56	122.68
1	B	522	ALA	CA-C-O	-5.60	115.03	121.19
1	B	251	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	261	GLU	N-CA-C	-5.60	99.39	108.41
1	B	215	SER	CA-C-O	-5.59	114.99	120.19
1	A	148	TRP	CE2-CD2-CG	-5.59	100.50	107.20
1	B	251	GLN	N-CA-C	-5.57	101.40	110.20
1	A	174	ILE	N-CA-C	-5.56	100.32	108.99
1	A	345	SER	CA-CB-OG	5.55	122.21	111.10
1	B	217	ARG	CA-CB-CG	5.55	125.20	114.10
1	A	529	GLN	O-C-N	5.55	129.56	123.01
1	B	451	LEU	CA-C-O	-5.55	115.00	120.82
1	A	147	GLU	N-CA-C	5.54	122.61	110.80
1	B	154	SER	CA-CB-OG	5.54	122.17	111.10
1	B	310	GLU	N-CA-C	-5.53	105.35	111.71
1	B	332	GLU	CA-CB-CG	5.53	125.16	114.10
1	B	461	ILE	N-CA-CB	-5.53	103.47	111.21
1	A	136	TYR	N-CA-C	-5.53	106.44	114.12
1	A	103	GLN	OE1-CD-NE2	-5.53	117.08	122.60
1	A	89	LEU	N-CA-C	5.52	119.18	112.23
1	B	507	PRO	O-C-N	-5.52	116.27	123.00
1	A	281	VAL	N-CA-C	-5.51	100.55	108.48
1	B	473	ARG	N-CA-C	-5.49	105.37	111.36
1	A	221	SER	CA-C-O	5.47	125.59	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	ASN	N-CA-C	-5.47	105.32	111.28
1	A	493	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	148	TRP	N-CA-C	5.44	120.20	113.50
1	B	284	ALA	N-CA-C	5.42	116.51	108.60
1	A	461	ILE	CA-C-N	5.41	125.17	119.76
1	A	461	ILE	C-N-CA	5.41	125.17	119.76
1	A	323	VAL	N-CA-C	5.41	115.05	107.37
1	A	124	LEU	N-CA-C	-5.39	105.50	111.71
1	A	125	ALA	N-CA-C	5.39	119.58	112.89
1	B	283	MET	CA-C-O	-5.39	115.68	121.56
1	B	143	LEU	CB-CA-C	-5.39	99.70	110.42
1	B	260	TRP	CE2-CD2-CG	-5.39	100.74	107.20
1	A	217	ARG	N-CA-C	5.38	120.80	113.37
1	B	500	LYS	CA-CB-CG	5.37	124.84	114.10
1	B	429	THR	CA-C-O	5.34	127.15	121.11
1	A	97	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	358	GLN	CB-CG-CD	5.33	121.66	112.60
1	B	282	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	B	148	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	B	483	ARG	CA-C-N	5.32	125.63	119.93
1	B	483	ARG	C-N-CA	5.32	125.63	119.93
1	A	497	ARG	CA-C-O	5.32	125.93	119.38
1	B	251	GLN	CB-CG-CD	5.29	121.60	112.60
1	B	254	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	B	500	LYS	N-CA-C	-5.29	100.78	109.40
1	B	106	ASP	N-CA-CB	5.27	117.90	110.36
1	B	396	ALA	O-C-N	5.27	127.57	122.09
1	A	392	ILE	N-CA-C	-5.26	100.90	108.48
1	B	118	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	A	495	MET	N-CA-C	5.26	117.43	111.11
1	B	188	VAL	CB-CA-C	-5.26	101.61	110.71
1	B	467	SER	CA-C-O	5.26	127.32	120.11
1	B	291	LYS	CA-C-O	-5.24	115.44	121.47
1	B	428	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	B	423	LYS	N-CA-C	-5.21	104.37	111.56
1	A	143	LEU	N-CA-C	5.20	121.87	110.80
1	B	327	ALA	N-CA-C	-5.17	101.41	108.38
1	B	140	VAL	O-C-N	5.16	127.94	122.67
1	A	270	GLU	O-C-N	-5.16	115.42	122.33
1	B	173	MET	CA-CB-CG	5.16	124.42	114.10
1	B	132	ILE	N-CA-CB	-5.16	103.99	111.21
1	A	503	PRO	CA-C-N	5.16	127.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	PRO	C-N-CA	5.16	127.44	120.38
1	B	218	SER	O-C-N	-5.15	117.55	123.42
1	B	301	SER	CB-CA-C	-5.15	101.10	110.63
1	B	510	GLU	CA-CB-CG	5.15	124.40	114.10
1	B	153	ILE	N-CA-C	5.15	115.69	108.89
1	B	143	LEU	CA-C-N	5.15	127.89	120.38
1	B	143	LEU	C-N-CA	5.15	127.89	120.38
1	A	489	GLU	CB-CG-CD	5.14	121.34	112.60
1	B	181	LYS	O-C-N	-5.14	116.93	122.79
1	A	201	HIS	CB-CG-ND1	5.14	130.41	122.70
1	A	239	GLN	N-CA-C	5.13	117.05	108.99
1	A	283	MET	CA-C-O	-5.13	115.75	121.81
1	B	440	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	175	ARG	O-C-N	5.12	128.60	122.72
1	B	118	TRP	CB-CG-CD1	-5.12	119.23	126.90
1	B	354	GLU	CA-C-N	5.11	125.61	119.94
1	B	354	GLU	C-N-CA	5.11	125.61	119.94
1	A	359	PRO	CB-CA-C	5.10	117.92	110.63
1	A	529	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	511	TYR	N-CA-C	-5.08	105.63	111.07
1	A	452	LEU	O-C-N	5.08	127.50	122.12
1	A	324	LYS	CG-CD-CE	5.08	122.97	111.30
1	A	381	ASN	N-CA-C	5.07	119.31	113.38
1	A	200	LYS	CA-CB-CG	-5.07	103.96	114.10
1	B	529	GLN	CA-C-N	5.07	130.92	121.69
1	B	529	GLN	C-N-CA	5.07	130.92	121.69
1	B	323	VAL	CB-CA-C	5.05	116.99	111.08
1	B	267	LEU	CA-C-O	5.05	126.87	121.16
1	B	181	LYS	N-CA-C	5.05	117.19	110.53
1	A	463	TYR	CA-CB-CG	5.04	122.96	113.90
1	A	466	MET	CA-C-O	5.04	126.69	121.15
1	B	278	PHE	CA-CB-CG	-5.04	108.76	113.80
1	B	510	GLU	CA-C-O	-5.03	115.21	120.55
1	B	96	HIS	CB-CG-ND1	5.02	130.23	122.70
1	A	262	ILE	CA-CB-CG2	5.02	119.03	110.50
1	A	295	LYS	N-CA-C	-5.01	100.36	108.52
1	B	529	GLN	N-CA-C	-5.01	102.29	110.20
1	B	93	GLU	CB-CG-CD	5.00	121.11	112.60
1	B	206	THR	CA-C-O	-5.00	115.15	120.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ASP	Peptide
1	B	192	ASP	Peptide
1	B	262	ILE	Peptide
1	B	458	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	3485	768	3422	103	0
1	B	3485	768	3422	87	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	10	1	0
3	B	22	0	10	1	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
All	All	7020	1536	6864	190	0

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

All (190) 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:A:322:LEU:HD23	1:A:402:ILE:HB	1.51	0.92
1:A:480:ARG:HD3	1:A:496:MET:HE1	1.50	0.92
1:B:388:ARG:HG3	1:B:390:ALA:HB3	1.65	0.78
1:A:191:TYR:HE1	1:A:193:PRO:HA	1.50	0.75
1:B:228:ASP:HA	1:B:231:LYS:HD3	1.69	0.73
1:B:372:GLU:HA	1:B:513:GLN:HE21	1.55	0.72
1:B:87:VAL:HB	1:B:140:VAL:HG22	1.71	0.72
1:A:295:LYS:HG2	1:A:297:MET:HE3	1.74	0.69
1:A:452:LEU:HB3	1:A:495:MET:HE2	1.74	0.69
1:A:302:MET:SD	1:A:307:PHE:HB2	2.32	0.69
1:B:450:ILE:O	1:B:453:MET:HB3	1.95	0.66
1:A:368:ALA:O	1:A:372:GLU:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:O	1:B:366:PHE:HB2	1.97	0.65
1:A:503:PRO:HA	1:A:506:ARG:HD2	1.80	0.64
1:A:480:ARG:NH1	1:A:499:TRP:HB3	2.13	0.64
1:A:347:LEU:O	1:A:351:LYS:HG3	1.98	0.63
1:A:326:HIS:HB2	1:A:337:ILE:O	1.99	0.63
1:B:457:THR:HB	1:B:460:ARG:HB3	1.80	0.63
1:A:87:VAL:O	1:A:137:VAL:HA	2.00	0.61
1:A:446:TRP:NE1	1:A:450:ILE:HD11	2.16	0.61
1:A:91:ASP:H	1:A:104:LYS:HZ3	1.49	0.61
1:B:480:ARG:HD3	1:B:496:MET:HE1	1.83	0.60
1:B:385:ARG:HH12	1:B:408:ALA:HB2	1.67	0.60
1:A:385:ARG:HH12	1:A:408:ALA:HB2	1.67	0.59
1:A:469:PRO:O	1:A:472:ILE:HG13	2.02	0.59
1:B:88:ALA:HA	1:B:137:VAL:HG12	1.83	0.59
1:A:426:ILE:HD13	1:A:427:LYS:HG3	1.84	0.59
1:A:123:SER:HB3	1:A:126:THR:OG1	2.02	0.58
1:B:150:PHE:CZ	1:B:245:CYS:HB3	2.39	0.58
1:B:295:LYS:HE3	1:B:297:MET:HE3	1.86	0.57
1:A:388:ARG:HG3	1:A:390:ALA:HB3	1.85	0.57
1:A:191:TYR:CE1	1:A:193:PRO:HA	2.35	0.57
1:A:113:GLU:HA	1:A:119:TRP:CD1	2.40	0.57
1:A:155:ARG:HG3	1:A:175:ARG:HH22	1.70	0.56
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.86	0.56
1:B:90:TYR:HA	1:B:104:LYS:HG2	1.88	0.56
1:A:262:ILE:HG22	1:A:329:VAL:HG22	1.88	0.56
1:A:155:ARG:HG3	1:A:175:ARG:NH2	2.21	0.56
1:B:108:MET:HG3	1:B:123:SER:HA	1.88	0.56
1:A:203:LYS:O	1:A:214:ILE:HG22	2.06	0.56
1:A:108:MET:HG3	1:A:123:SER:HA	1.88	0.55
1:A:153:ILE:HG22	1:A:154:SER:O	2.07	0.55
1:B:372:GLU:HA	1:B:513:GLN:NE2	2.21	0.55
1:A:474:ALA:HB1	1:A:479:TYR:HB3	1.89	0.55
1:A:495:MET:O	1:A:498:CYS:HB2	2.06	0.55
1:A:325:LEU:HD22	1:A:338:THR:HG22	1.88	0.54
1:A:405:PHE:CD1	1:A:405:PHE:N	2.75	0.54
1:A:224:GLN:O	1:A:227:VAL:HG22	2.07	0.54
1:A:84:ILE:H	1:A:84:ILE:HD12	1.72	0.54
1:B:272:LYS:HE2	1:B:282:TRP:HZ2	1.73	0.53
1:B:446:TRP:CZ3	1:B:499:TRP:HA	2.43	0.53
1:B:469:PRO:O	1:B:472:ILE:HG13	2.09	0.53
1:B:442:LYS:HD2	1:B:503:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TRP:HE1	1:A:450:ILE:HD11	1.73	0.53
1:A:450:ILE:O	1:A:453:MET:HB3	2.08	0.53
1:B:319:HIS:HB3	1:B:322:LEU:HG	1.91	0.53
1:A:168:MET:O	1:A:189:ARG:HD2	2.08	0.53
1:B:374:MET:HE2	1:B:387:LEU:HD11	1.89	0.52
1:A:322:LEU:CD2	1:A:402:ILE:HB	2.31	0.52
1:A:449:GLY:O	1:A:452:LEU:HB2	2.10	0.52
1:B:452:LEU:HD13	1:B:491:LEU:HD11	1.90	0.52
1:A:405:PHE:N	1:A:405:PHE:HD1	2.08	0.52
1:B:453:MET:HG2	1:B:481:MET:HE3	1.92	0.52
1:A:226:LEU:O	1:A:229:HIS:HB3	2.10	0.52
1:B:87:VAL:HG12	1:B:138:ALA:O	2.10	0.52
1:A:484:PRO:HB2	1:A:487:CYS:HB2	1.92	0.51
1:B:371:ALA:O	1:B:374:MET:HB2	2.11	0.51
1:A:191:TYR:HD1	1:A:192:ASP:N	2.08	0.51
1:B:174:ILE:HD11	1:B:227:VAL:HG12	1.92	0.51
1:A:310:GLU:O	1:A:313:VAL:HB	2.11	0.51
1:B:206:THR:HG22	1:B:212:PHE:HD2	1.76	0.51
1:B:468:ASN:O	1:B:471:VAL:HG22	2.11	0.50
1:B:191:TYR:HE1	1:B:193:PRO:HA	1.76	0.50
1:B:397:SER:O	1:B:398:LEU:HB2	2.10	0.50
1:B:448:PHE:CE1	1:B:452:LEU:HD21	2.46	0.50
1:A:169:LEU:H	1:A:169:LEU:HD12	1.75	0.50
1:B:424:PHE:O	1:B:426:ILE:HG13	2.12	0.49
1:B:448:PHE:CZ	1:B:452:LEU:HD21	2.47	0.49
1:A:150:PHE:HD2	1:A:173:MET:HB2	1.77	0.49
1:A:203:LYS:HD3	1:B:489:GLU:HG2	1.94	0.49
1:A:346:LEU:O	1:A:349:PHE:HB3	2.14	0.48
1:B:123:SER:HB3	1:B:126:THR:OG1	2.13	0.48
1:B:184:TYR:O	1:B:204:ILE:HB	2.13	0.48
1:B:310:GLU:O	1:B:313:VAL:HB	2.13	0.48
1:A:489:GLU:HG2	1:B:203:LYS:HD3	1.95	0.48
1:B:84:ILE:HD13	1:B:110:VAL:HG13	1.96	0.48
1:A:264:ARG:NH2	1:A:333:PRO:O	2.47	0.48
1:A:262:ILE:O	1:A:329:VAL:HG13	2.13	0.48
1:B:204:ILE:HA	1:B:214:ILE:HG22	1.96	0.48
1:B:382:TYR:OH	1:B:406:GLY:HA3	2.13	0.48
1:A:330:THR:HB	1:A:331:LYS:HZ3	1.80	0.47
1:B:177:SER:HB2	1:B:180:THR:O	2.14	0.47
1:A:374:MET:HE2	1:A:387:LEU:CD1	2.45	0.47
1:B:384:HIS:ND1	1:B:405:PHE:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LYS:HE2	1:B:282:TRP:CZ2	2.48	0.47
1:A:323:VAL:HG13	1:A:323:VAL:O	2.14	0.47
1:B:89:LEU:HB3	1:B:90:TYR:CD2	2.49	0.47
1:A:329:VAL:O	1:A:334:ILE:HG23	2.15	0.47
1:B:428:TRP:HE1	1:B:454:GLU:CD	2.23	0.47
1:A:213:TYR:HD2	1:A:215:SER:O	1.98	0.46
1:A:330:THR:HB	1:A:331:LYS:NZ	2.30	0.46
1:A:430:ALA:HB2	1:A:446:TRP:HB3	1.97	0.46
1:A:121:ALA:HB3	1:A:132:ILE:HD13	1.97	0.46
1:B:363:LEU:HD23	1:B:455:ILE:HG22	1.97	0.46
1:B:480:ARG:NH1	1:B:499:TRP:HB3	2.29	0.46
1:A:280:GLU:HB2	1:A:296:THR:OG1	2.14	0.46
1:B:90:TYR:HB2	1:B:136:TYR:CD2	2.51	0.46
1:A:91:ASP:OD1	1:A:104:LYS:HG3	2.15	0.46
1:A:374:MET:HE2	1:A:387:LEU:HD11	1.97	0.46
1:A:272:LYS:HE2	1:A:282:TRP:CZ2	2.50	0.46
1:A:262:ILE:HA	1:A:263:PRO:HD2	1.78	0.46
1:A:480:ARG:NH1	1:A:499:TRP:O	2.49	0.46
3:A:1:QUE:H15	3:A:1:QUE:O27	2.15	0.46
1:A:223:LEU:O	1:A:227:VAL:HG13	2.16	0.46
1:B:474:ALA:HA	1:B:477:ARG:HG2	1.98	0.46
1:B:262:ILE:HA	1:B:263:PRO:HD2	1.68	0.46
1:A:463:TYR:HB3	1:A:466:MET:HG3	1.97	0.46
1:B:501:ASN:O	1:B:503:PRO:HD3	2.16	0.46
1:B:405:PHE:CD1	1:B:405:PHE:N	2.84	0.45
1:B:466:MET:SD	1:B:471:VAL:HG12	2.55	0.45
1:B:89:LEU:HD13	1:B:89:LEU:HA	1.77	0.45
1:B:214:ILE:HD11	1:B:237:LEU:HD21	1.98	0.45
1:A:211:GLY:HA2	1:A:221:SER:HA	1.97	0.45
1:B:347:LEU:HB2	1:B:389:ALA:HB3	1.97	0.45
1:A:442:LYS:HD2	1:A:503:PRO:O	2.17	0.45
1:B:431:PRO:HA	1:B:434:ILE:HD12	1.98	0.45
1:A:448:PHE:HE1	1:A:452:LEU:HD11	1.81	0.45
1:A:530:GLN:HA	1:A:531:PRO:HD3	1.81	0.45
1:B:204:ILE:HG12	1:B:214:ILE:CG2	2.47	0.44
1:B:492:TYR:O	1:B:495:MET:HB2	2.17	0.44
1:A:487:CYS:SG	1:A:491:LEU:HD23	2.57	0.44
1:A:488:PRO:HG2	1:A:491:LEU:HB2	2.00	0.44
1:A:109:VAL:O	1:A:121:ALA:HA	2.18	0.44
1:A:119:TRP:HB2	1:A:132:ILE:HG22	1.99	0.44
1:A:286:TYR:HB3	1:A:290:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:HA	1:B:119:TRP:CD1	2.53	0.44
1:B:171:SER:HA	1:B:243:VAL:O	2.17	0.44
1:A:220:PHE:HZ	1:A:229:HIS:ND1	2.15	0.43
1:B:91:ASP:OD1	1:B:104:LYS:HG3	2.18	0.43
1:B:363:LEU:HD23	1:B:455:ILE:CG2	2.48	0.43
1:B:213:TYR:HB3	1:B:219:THR:HG23	2.00	0.43
1:B:109:VAL:O	1:B:121:ALA:HA	2.19	0.43
1:A:214:ILE:HG13	1:A:215:SER:H	1.84	0.43
1:A:480:ARG:HH11	1:A:499:TRP:HB3	1.84	0.43
1:A:87:VAL:HB	1:A:140:VAL:HG22	2.01	0.43
1:A:306:ALA:O	1:A:309:ALA:HB3	2.19	0.43
1:A:450:ILE:HD13	1:A:499:TRP:CZ2	2.53	0.43
1:B:222:THR:HB	1:B:225:GLU:CB	2.48	0.43
1:B:262:ILE:HA	1:B:262:ILE:HD13	1.66	0.43
1:A:122:ARG:HA	1:A:129:GLU:HA	2.00	0.43
1:A:453:MET:HE2	1:A:495:MET:SD	2.59	0.43
1:B:189:ARG:HG2	1:B:190:ASP:N	2.33	0.43
1:B:153:ILE:HG22	1:B:154:SER:O	2.19	0.43
1:B:453:MET:O	1:B:457:THR:HG23	2.19	0.43
1:A:307:PHE:CE2	1:A:328:VAL:HG21	2.54	0.42
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.88	0.42
1:A:168:MET:SD	1:A:242:SER:HB2	2.58	0.42
1:B:429:THR:HG22	1:B:433:ALA:HB3	1.99	0.42
3:B:532:QUE:H5	4:B:534:HOH:O	2.19	0.42
1:A:262:ILE:HA	1:A:262:ILE:HD13	1.61	0.42
1:A:445:VAL:O	1:A:446:TRP:C	2.62	0.42
1:B:347:LEU:O	1:B:351:LYS:HG3	2.19	0.42
1:A:447:SER:O	1:A:450:ILE:N	2.51	0.42
1:B:450:ILE:HD13	1:B:499:TRP:CZ2	2.55	0.42
1:B:224:GLN:O	1:B:227:VAL:HG22	2.19	0.42
1:B:334:ILE:H	1:B:334:ILE:HD12	1.85	0.42
1:B:172:PHE:HB3	1:B:188:VAL:HG13	2.01	0.42
1:A:307:PHE:HE2	1:A:328:VAL:HG21	1.85	0.42
1:B:293:ALA:O	1:B:337:ILE:HA	2.20	0.42
1:B:279:GLY:HA2	1:B:296:THR:O	2.20	0.42
1:A:374:MET:HB3	1:A:509:PHE:CG	2.55	0.41
1:A:450:ILE:HD13	1:A:499:TRP:CE2	2.55	0.41
1:A:500:LYS:HB3	1:A:506:ARG:HG3	2.01	0.41
1:B:132:ILE:HA	1:B:133:PRO:HD2	1.81	0.41
1:B:487:CYS:SG	1:B:488:PRO:HD2	2.60	0.41
1:A:501:ASN:O	1:A:503:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD23	1:A:456:VAL:HA	2.03	0.41
1:A:167:ASN:HB2	1:A:189:ARG:NH2	2.36	0.41
1:A:90:TYR:HA	1:A:104:LYS:HG2	2.03	0.41
1:A:118:TRP:HA	1:A:132:ILE:O	2.20	0.41
1:A:385:ARG:NH1	1:A:408:ALA:HB2	2.34	0.41
1:A:427:LYS:HD3	1:A:462:PRO:O	2.21	0.41
1:A:504:GLU:H	1:A:504:GLU:CD	2.29	0.41
1:A:435:ASN:HB2	1:A:436:PHE:CD2	2.56	0.41
1:B:433:ALA:HA	1:B:438:SER:O	2.21	0.41
1:A:186:LEU:O	1:A:201:HIS:HA	2.21	0.40
1:A:500:LYS:HB3	1:A:506:ARG:CG	2.51	0.40
1:B:84:ILE:H	1:B:84:ILE:HD12	1.86	0.40
1:B:226:LEU:O	1:B:230:TYR:HD2	2.04	0.40
1:B:321:LYS:O	1:B:322:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/438 (99%)	380 (88%)	41 (10%)	12 (3%)	4	21
1	B	433/438 (99%)	388 (90%)	35 (8%)	10 (2%)	5	25
All	All	866/876 (99%)	768 (89%)	76 (9%)	22 (2%)	4	23

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLU
1	A	425	PRO
1	A	426	ILE
1	A	434	ILE

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Mol	Chain	Res	Type
1	A	468	ASN
1	B	147	GLU
1	B	426	ILE
1	B	468	ASN
1	B	196	GLY
1	B	292	VAL
1	B	385	ARG
1	A	143	LEU
1	A	264	ARG
1	A	288	LYS
1	A	385	ARG
1	B	425	PRO
1	A	151	LYS
1	B	151	LYS
1	B	244	PRO
1	A	503	PRO
1	B	434	ILE
1	A	292	VAL

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	369/382 (97%)	320 (87%)	49 (13%)	4	18
1	B	369/382 (97%)	311 (84%)	58 (16%)	2	13
All	All	738/764 (97%)	631 (86%)	107 (14%)	3	15

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	85	ILE
1	A	93	GLU
1	A	98	GLU
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	103	GLN
1	A	108	MET
1	A	110	VAL
1	A	124	LEU
1	A	132	ILE
1	A	134	SER
1	A	188	VAL
1	A	191	TYR
1	A	205	ARG
1	A	212	PHE
1	A	222	THR
1	A	223	LEU
1	A	224	GLN
1	A	227	VAL
1	A	242	SER
1	A	246	MET
1	A	247	SER
1	A	248	SER
1	A	262	ILE
1	A	269	LEU
1	A	271	LYS
1	A	290	THR
1	A	294	VAL
1	A	312	ASN
1	A	324	LYS
1	A	325	LEU
1	A	330	THR
1	A	331	LYS
1	A	347	LEU
1	A	358	GLN
1	A	367	SER
1	A	384	HIS
1	A	387	LEU
1	A	397	SER
1	A	405	PHE
1	A	426	ILE
1	A	432	GLU
1	A	440	THR
1	A	443	SER
1	A	450	ILE
1	A	468	ASN
1	A	480	ARG

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Mol	Chain	Res	Type
1	A	500	LYS
1	A	503	PRO
1	B	84	ILE
1	B	85	ILE
1	B	89	LEU
1	B	93	GLU
1	B	98	GLU
1	B	100	LEU
1	B	106	ASP
1	B	108	MET
1	B	110	VAL
1	B	124	LEU
1	B	132	ILE
1	B	134	SER
1	B	168	MET
1	B	188	VAL
1	B	198	THR
1	B	205	ARG
1	B	212	PHE
1	B	221	SER
1	B	222	THR
1	B	223	LEU
1	B	224	GLN
1	B	227	VAL
1	B	244	PRO
1	B	246	MET
1	B	248	SER
1	B	251	GLN
1	B	257	LYS
1	B	262	ILE
1	B	267	LEU
1	B	269	LEU
1	B	281	VAL
1	B	283	MET
1	B	290	THR
1	B	317	LEU
1	B	323	VAL
1	B	324	LYS
1	B	325	LEU
1	B	330	THR
1	B	331	LYS
1	B	336	ILE

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Mol	Chain	Res	Type
1	B	358	GLN
1	B	387	LEU
1	B	388	ARG
1	B	405	PHE
1	B	426	ILE
1	B	429	THR
1	B	432	GLU
1	B	440	THR
1	B	441	ILE
1	B	443	SER
1	B	466	MET
1	B	472	ILE
1	B	480	ARG
1	B	483	ARG
1	B	493	ASN
1	B	500	LYS
1	B	508	THR
1	B	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	103	GLN
1	A	161	GLN
1	A	251	GLN
1	B	103	GLN
1	B	161	GLN
1	B	251	GLN
1	B	391	ASN
1	B	501	ASN
1	B	513	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	PTR	A	527	2,1	15,16,17	1.31	1 (6%)	17,22,24	2.05	7 (41%)
1	PTR	B	527	2,1	15,16,17	1.07	1 (6%)	17,22,24	1.24	2 (11%)

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
1	PTR	A	527	2,1	-	1/10/11/13	0/1/1/1
1	PTR	B	527	2,1	-	2/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	CB-CA	-3.09	1.47	1.53
1	B	527	PTR	P-O3P	-2.37	1.46	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PTR	OH-CZ-CE2	-3.49	108.75	119.22
1	A	527	PTR	CB-CG-CD2	-3.31	114.74	120.90
1	A	527	PTR	O2P-P-OH	3.15	114.63	105.32
1	A	527	PTR	OH-CZ-CE1	2.90	127.91	119.22
1	A	527	PTR	CD1-CE1-CZ	-2.88	116.44	119.73
1	B	527	PTR	O2P-P-OH	2.83	113.67	105.32
1	A	527	PTR	CE2-CZ-CE1	2.18	123.34	120.16
1	B	527	PTR	CD2-CG-CD1	2.06	121.30	118.23
1	A	527	PTR	CD2-CG-CD1	2.02	121.24	118.23

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	PTR	O-C-CA-CB
1	B	527	PTR	N-CA-CB-CG
1	B	527	PTR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	QUE	A	1	-	24,24,24	2.21	5 (20%)	36,36,36	2.71	14 (38%)
3	QUE	B	532	-	24,24,24	2.56	11 (45%)	36,36,36	3.37	21 (58%)

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	QUE	A	1	-	-	0/4/4/4	0/3/3/3
3	QUE	B	532	-	-	0/4/4/4	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	532	QUE	C10-C11	8.27	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	QUE	C10-C11	7.88	1.44	1.36
3	B	532	QUE	C14-C11	-4.05	1.41	1.47
3	B	532	QUE	C1-C2	3.43	1.43	1.38
3	A	1	QUE	C1-C2	2.96	1.43	1.38
3	B	532	QUE	O12-C4	-2.72	1.34	1.38
3	A	1	QUE	C14-C11	-2.72	1.43	1.47
3	B	532	QUE	O27-C10	2.68	1.42	1.33
3	B	532	QUE	C3-C2	2.58	1.45	1.41
3	B	532	QUE	O24-C17	2.41	1.41	1.36
3	B	532	QUE	C16-C15	2.35	1.42	1.38
3	B	532	QUE	C16-C17	2.32	1.43	1.39
3	A	1	QUE	O24-C17	2.16	1.40	1.36
3	A	1	QUE	O23-C18	2.16	1.40	1.36
3	B	532	QUE	O23-C18	2.14	1.40	1.36
3	B	532	QUE	C1-C6	2.00	1.42	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	532	QUE	C11-C10-C9	-10.95	113.70	121.52
3	B	532	QUE	C14-C19-C18	7.07	126.26	120.09
3	A	1	QUE	C14-C19-C18	6.77	125.99	120.09
3	A	1	QUE	C11-C10-C9	-5.67	117.47	121.52
3	B	532	QUE	C2-C3-C4	-5.29	112.35	117.41
3	A	1	QUE	O12-C11-C14	4.92	117.76	110.87
3	B	532	QUE	O27-C10-C11	4.75	125.65	120.74
3	B	532	QUE	C15-C14-C11	4.71	127.64	120.71
3	B	532	QUE	C2-C3-C9	4.53	128.15	121.45
3	A	1	QUE	C14-C11-C10	-4.39	121.53	128.44
3	A	1	QUE	C2-C1-C6	4.36	123.70	119.67
3	A	1	QUE	C15-C14-C11	4.33	127.08	120.71
3	B	532	QUE	C5-C6-C1	-4.19	114.72	120.47
3	A	1	QUE	C15-C14-C19	-3.90	114.73	119.25
3	A	1	QUE	C5-C6-C1	-3.84	115.21	120.47
3	B	532	QUE	C2-C1-C6	3.72	123.11	119.67
3	B	532	QUE	C19-C14-C11	-3.45	115.78	120.65
3	B	532	QUE	C14-C11-C10	-3.41	123.07	128.44
3	B	532	QUE	C19-C18-C17	-3.23	116.90	119.89
3	A	1	QUE	O12-C4-C3	-3.19	118.06	121.19
3	B	532	QUE	C3-C9-C10	3.16	121.35	116.88
3	B	532	QUE	O12-C4-C3	-3.11	118.14	121.19
3	A	1	QUE	O27-C10-C11	2.96	123.80	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	532	QUE	C4-O12-C11	2.89	125.10	120.67
3	B	532	QUE	O12-C11-C14	2.69	114.64	110.87
3	A	1	QUE	O23-C18-C17	2.63	125.44	118.42
3	A	1	QUE	C19-C18-C17	-2.62	117.46	119.89
3	B	532	QUE	C4-C5-C6	2.58	123.05	118.98
3	A	1	QUE	C2-C3-C4	-2.55	114.97	117.41
3	B	532	QUE	O29-C6-C1	2.50	126.40	119.85
3	B	532	QUE	O23-C18-C17	2.41	124.85	118.42
3	B	532	QUE	C15-C14-C19	-2.40	116.47	119.25
3	B	532	QUE	O12-C11-C10	2.17	122.25	120.19
3	B	532	QUE	O27-C10-C9	2.04	120.65	116.89
3	A	1	QUE	O24-C17-C18	2.04	123.87	118.42

There are no chirality outliers.

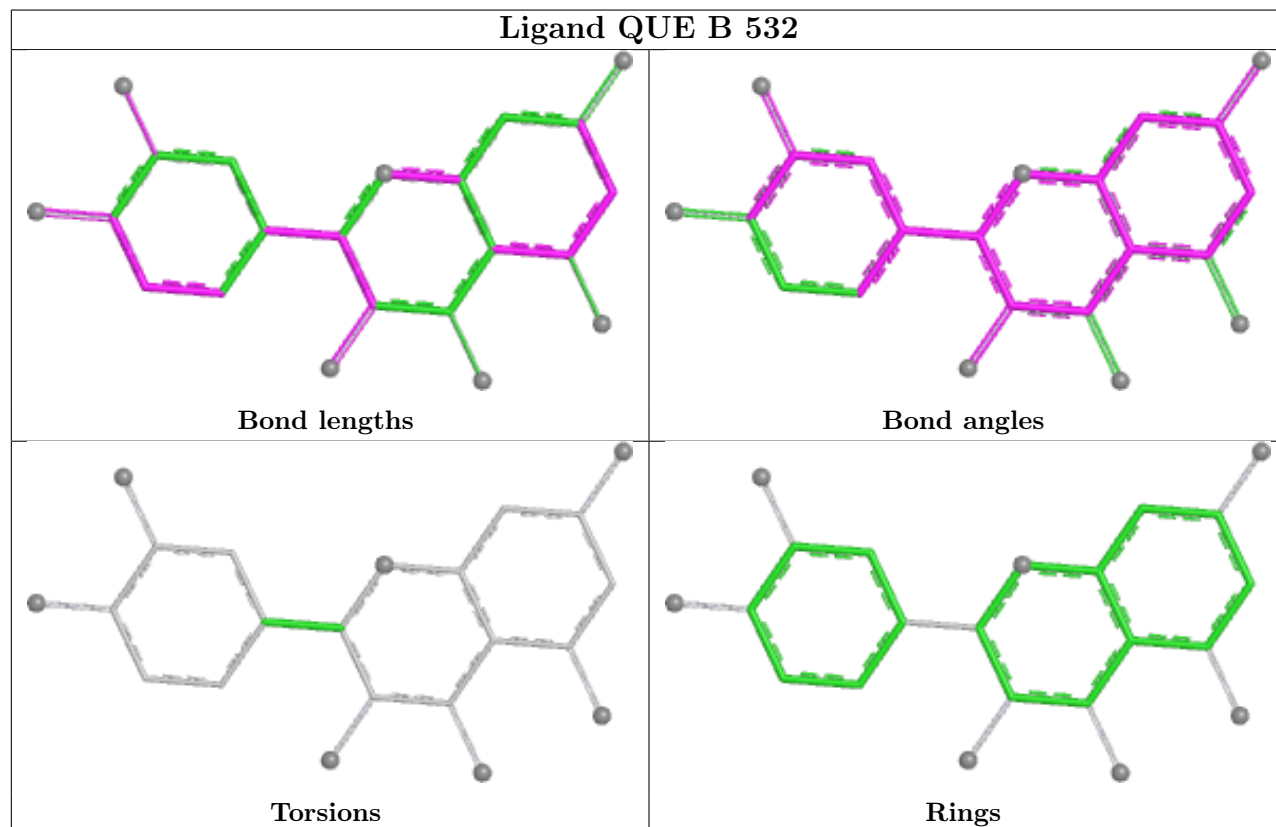
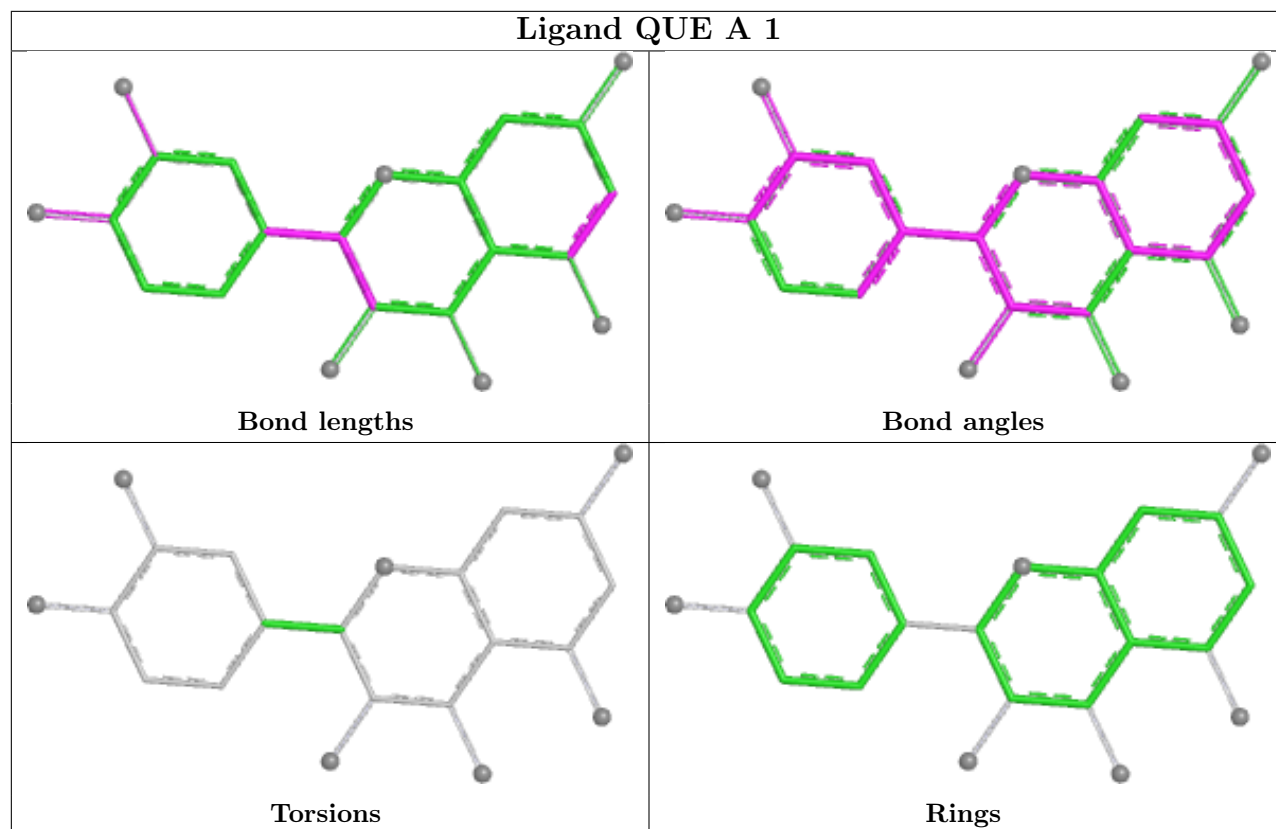
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	QUE	1	0
3	B	532	QUE	1	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	411:GLY	C	422:ALA	N	9.40
1	B	411:GLY	C	422:ALA	N	9.39

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.