Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:28 pm BST

PDB ID	:	2HCK
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 following versions of software and data (see references ⓘ) were used in the production of this report:

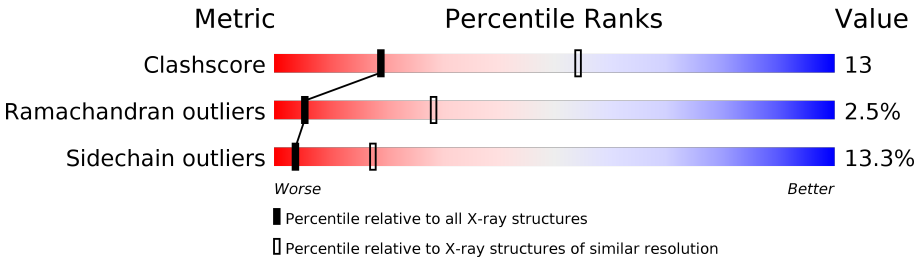
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 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	438	59% 31% 9%
1	B	438	55% 36% 7%

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			

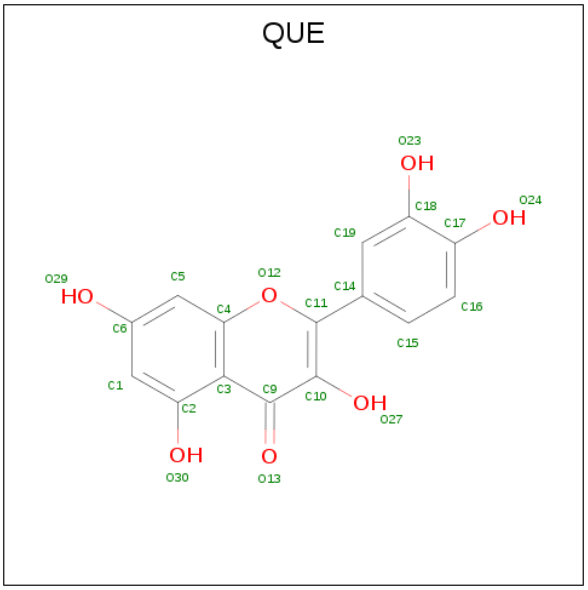
There are 22 discrepancies between the modelled and reference sequences:

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (three-letter code: QUE) (formula: $C_{15}H_{10}O_7$).



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

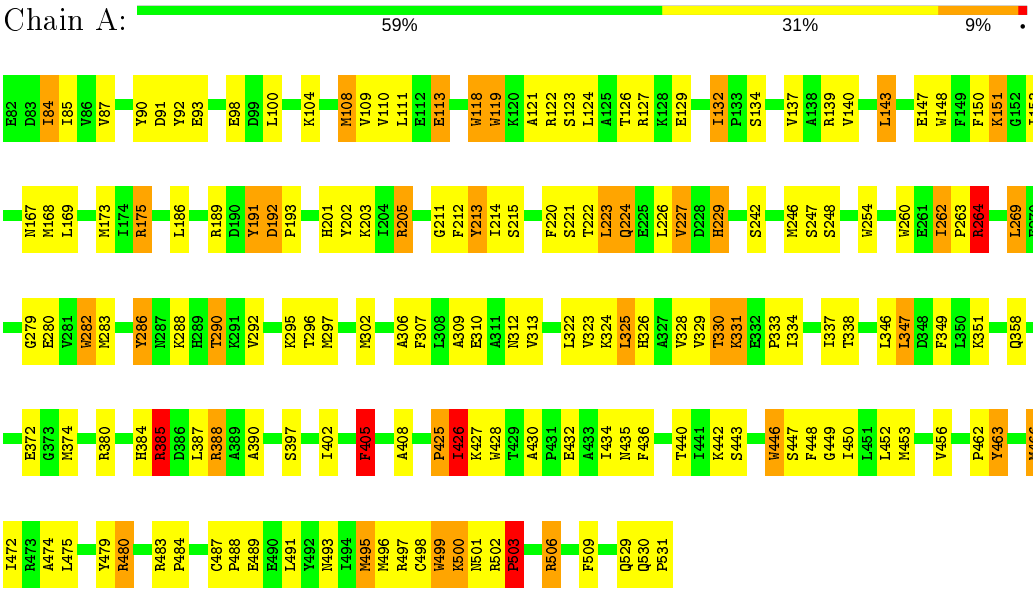
3 Residue-property plots (i)

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.

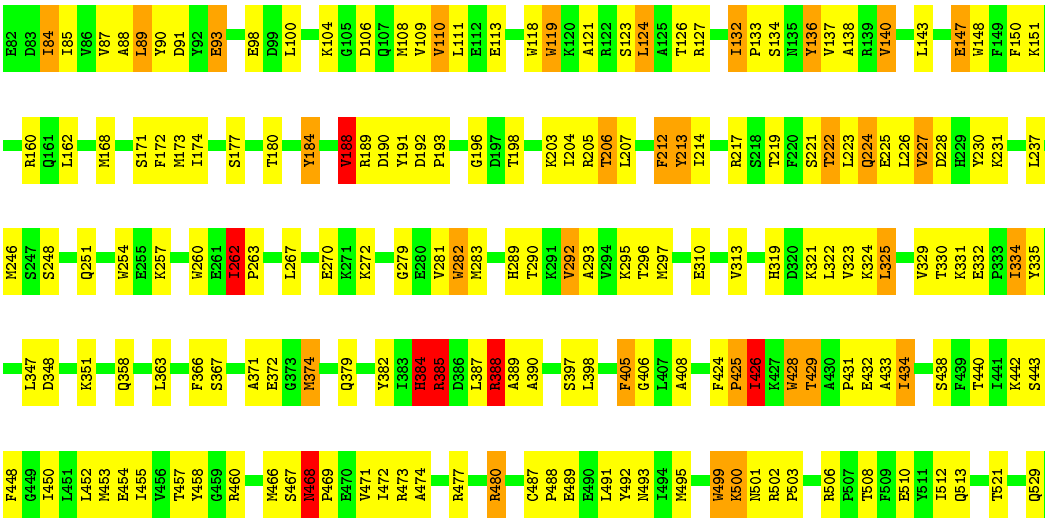
- Molecule 1: HEMATOPOETIC CELL KINASE HCK

Chain A:



- Molecule 1: HEMATOPOETIC CELL KINASE HCK

Chain B:



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	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	0.99	0/3552	1.71	67/4799 (1.4%)
1	B	1.00	0/3552	1.77	77/4799 (1.6%)
All	All	1.00	0/7104	1.74	144/9598 (1.5%)

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

There are no bond length outliers.

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	A	283	MET	CG-SD-CE	-10.61	83.22	100.20
1	A	127	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	264	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	B	282	TRP	CD1-CG-CD2	9.62	113.99	106.30
1	A	506	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	B	260	TRP	CD1-CG-CD2	9.28	113.72	106.30
1	A	160	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	497	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	202	TYR	CB-CG-CD2	-8.71	115.77	121.00
1	A	118	TRP	CD1-CG-CD2	8.68	113.24	106.30
1	A	148	TRP	CD1-CG-CD2	8.60	113.18	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	TRP	CE2-CD2-CG	-8.51	100.50	107.30
1	B	254	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	B	118	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	B	260	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	B	374	MET	CA-CB-CG	-8.12	99.50	113.30
1	B	282	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	B	254	TRP	CE2-CD2-CG	-8.06	100.85	107.30
1	B	118	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	B	160	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	B	499	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	A	148	TRP	CG-CD2-CE3	7.69	140.82	133.90
1	A	388	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	428	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	A	118	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	A	254	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	B	119	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	A	160	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	160	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	428	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	A	425	PRO	N-CA-C	7.36	131.24	112.10
1	A	502	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	119	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	428	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	282	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	B	148	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	139	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	254	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	499	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	B	467	SER	CA-C-N	-7.15	101.47	117.20
1	A	119	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	B	124	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	446	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	260	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	446	TRP	CE2-CD2-CG	-6.96	101.74	107.30
1	B	213	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	B	428	TRP	CD1-CG-CD2	6.92	111.84	106.30
1	B	446	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	119	TRP	CE2-CD2-CG	-6.91	101.78	107.30
1	B	499	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	B	148	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	148	TRP	CB-CG-CD1	-6.74	118.23	127.00
1	B	127	ARG	NE-CZ-NH2	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	118	TRP	CG-CD2-CE3	6.65	139.88	133.90
1	A	175	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	173	MET	CA-CB-CG	6.54	124.42	113.30
1	B	512	ILE	CG1-CB-CG2	-6.51	97.07	111.40
1	A	139	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	282	TRP	CE2-CD2-CG	-6.41	102.17	107.30
1	A	286	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	A	380	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	385	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	495	MET	CG-SD-CE	-6.30	90.11	100.20
1	B	207	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	499	TRP	CD1-CG-CD2	6.17	111.23	106.30
1	B	367	SER	CA-CB-OG	-6.12	94.67	111.20
1	A	205	ARG	CB-CG-CD	6.04	127.31	111.60
1	B	118	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	B	148	TRP	CG-CD2-CE3	5.92	139.22	133.90
1	B	468	ASN	CA-C-N	5.83	133.42	117.10
1	B	428	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	B	384	HIS	N-CA-C	-5.80	95.33	111.00
1	B	140	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	A	502	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	428	TRP	CB-CG-CD1	-5.73	119.55	127.00
1	B	270	GLU	CA-C-N	5.72	129.79	117.20
1	B	270	GLU	O-C-N	-5.72	113.55	122.70
1	A	446	TRP	CD1-CG-CD2	5.71	110.87	106.30
1	B	388	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	93	GLU	N-CA-C	-5.67	95.69	111.00
1	B	206	THR	CA-C-N	5.67	129.68	117.20
1	A	260	TRP	CD1-CG-CD2	5.65	110.82	106.30
1	A	276	GLY	N-CA-C	-5.65	98.98	113.10
1	B	283	MET	CG-SD-CE	-5.63	91.19	100.20
1	A	405	PHE	CB-CG-CD1	5.63	124.74	120.80
1	B	444	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	184	TYR	O-C-N	-5.59	113.75	122.70
1	B	148	TRP	CB-CG-CD1	-5.58	119.75	127.00
1	A	506	ARG	CB-CG-CD	-5.53	97.21	111.60
1	B	143	LEU	CB-CA-C	-5.53	99.70	110.20
1	B	506	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	155	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	111	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	506	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	147	GLU	N-CA-C	5.43	125.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	466	MET	CA-C-N	-5.42	105.28	117.20
1	A	143	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	229	HIS	CA-CB-CG	5.40	122.77	113.60
1	A	260	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	B	425	PRO	N-CA-C	5.39	126.13	112.10
1	B	217	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	143	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	475	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	151	LYS	N-CA-C	5.37	125.49	111.00
1	B	217	ARG	CA-CB-CG	5.37	125.20	113.40
1	A	385	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	332	GLU	CA-CB-CG	5.35	125.16	113.40
1	A	428	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	B	143	LEU	N-CA-C	5.33	125.38	111.00
1	A	113	GLU	CA-CB-CG	-5.32	101.71	113.40
1	A	529	GLN	CA-C-N	-5.31	105.52	117.20
1	B	254	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	148	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	A	483	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	282	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	260	TRP	CG-CD2-CE3	5.26	138.64	133.90
1	B	502	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	254	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	B	136	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	374	MET	N-CA-CB	-5.24	101.16	110.60
1	B	155	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	151	LYS	CA-C-N	5.24	126.67	116.20
1	B	260	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	341	MET	CA-C-N	-5.23	105.69	117.20
1	A	428	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	A	269	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	500	LYS	CA-CB-CG	5.20	124.84	113.40
1	B	111	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	188	VAL	CB-CA-C	-5.16	101.61	111.40
1	A	92	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	325	LEU	O-C-N	-5.12	114.51	122.70
1	B	289	HIS	CA-CB-CG	5.10	122.27	113.60
1	B	388	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	473	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	140	VAL	CA-C-N	-5.06	106.06	117.20
1	A	279	GLY	CA-C-N	-5.06	106.08	117.20
1	A	380	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	A	254	TRP	CG-CD2-CE3	5.04	138.44	133.90
1	A	463	TYR	CA-CB-CG	5.03	122.96	113.40
1	B	529	GLN	O-C-N	5.02	130.73	122.70
1	B	292	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	B	510	GLU	CA-CB-CG	5.00	124.40	113.40

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	96	0
1	B	3485	768	3422	84	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	180	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 13.

All (180) 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: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:302:MET:SD	1:A:307:PHE:HB2	2.32	0.69
1:A:295:LYS:HG2	1:A:297:MET:HE3	1.73	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
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: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: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:B:295:LYS:HE3	1:B:297:MET:HE3	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:91:ASP:H	1:A:104:LYS:HZ3	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD22	1:A:338:THR:HG22	1.88	0.54
1:A:405:PHE:N	1:A:405:PHE:CD1	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:469:PRO:O	1:B:472:ILE:HG13	2.09	0.53
1:B:446:TRP:CZ3	1:B:499:TRP:HA	2.43	0.53
1:B:442:LYS:HD2	1:B:503:PRO:O	2.08	0.53
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: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: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:397:SER:O	1:B:398:LEU:HB2	2.10	0.50
1:B:191:TYR:HE1	1:B:193:PRO:HA	1.76	0.50
1:B:448:PHE:CE1	1:B:452:LEU:HD21	2.46	0.50
1:A:169:LEU:HD12	1:A:169:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:177:SER:HB2	1:B:180:THR:O	2.14	0.47
1:B:384:HIS:ND1	1:B:405:PHE:HA	2.30	0.47
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: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:272:LYS:HE2	1:A:282:TRP:CZ2	2.50	0.46
3:A:1:QUE:H15	3:A:1:QUE:O27	2.15	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
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:214:ILE:HD11	1:B:237:LEU:HD21	1.98	0.45
1:B:89:LEU:HA	1:B:89:LEU:HD13	1.77	0.45
1:A:211:GLY:HA2	1:A:221:SER:HA	1.97	0.45
1:A:480:ARG:HD3	1:A:496:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:363:LEU:HD23	1:B:455:ILE:CG2	2.48	0.43
1:B:91:ASP:OD1	1:B:104:LYS:HG3	2.18	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: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:A:87:VAL:HB	1:A:140:VAL:HG22	2.01	0.43
1:B:222:THR:HB	1:B:225:GLU:CB	2.48	0.43
1:B:262:ILE:HD13	1:B:262:ILE:HA	1.66	0.43
1:A:122:ARG:HA	1:A:129:GLU:HA	2.00	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:HA	1:B:162:LEU:HD23	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:HD13	1:A:262:ILE:HA	1.61	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:HD12	1:B:334:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASN:O	1:A:503:PRO:HD3	2.20	0.41
1:B:428:TRP:HE1	1:B:454:GLU:CD	2.23	0.41
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: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:226:LEU:O	1:B:230:TYR:HD2	2.04	0.40
1:B:84:ILE:HD12	1:B:84:ILE:H	1.86	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	433/438 (99%)	380 (88%)	41 (10%)	12 (3%)	5 25
1	B	433/438 (99%)	388 (90%)	35 (8%)	10 (2%)	6 30
All	All	866/876 (99%)	768 (89%)	76 (9%)	22 (2%)	5 28

All (22) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	434	ILE
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 (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	369/382 (97%)	323 (88%)	46 (12%)	4 20
1	B	369/382 (97%)	317 (86%)	52 (14%)	3 16
All	All	738/764 (97%)	640 (87%)	98 (13%)	4 17

All (98) 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

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Mol	Chain	Res	Type
1	A	100	LEU
1	A	108	MET
1	A	110	VAL
1	A	124	LEU
1	A	132	ILE
1	A	134	SER
1	A	191	TYR
1	A	205	ARG
1	A	212	PHE
1	A	213	TYR
1	A	222	THR
1	A	223	LEU
1	A	224	GLN
1	A	227	VAL
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	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	468	ASN
1	A	480	ARG
1	A	493	ASN
1	A	500	LYS
1	A	503	PRO

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Mol	Chain	Res	Type
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	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	281	VAL
1	B	290	THR
1	B	323	VAL
1	B	324	LYS
1	B	325	LEU
1	B	330	THR
1	B	331	LYS
1	B	348	ASP
1	B	358	GLN
1	B	379	GLN
1	B	384	HIS
1	B	387	LEU
1	B	388	ARG
1	B	405	PHE

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Mol	Chain	Res	Type
1	B	426	ILE
1	B	429	THR
1	B	432	GLU
1	B	440	THR
1	B	443	SER
1	B	480	ARG
1	B	493	ASN
1	B	500	LYS
1	B	508	THR
1	B	521	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	513	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1,2	15,16,17	1.26	1 (6%)	19,22,24	1.91	6 (31%)
1	PTR	B	527	1,2	15,16,17	1.09	1 (6%)	19,22,24	1.51	2 (10%)

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	1,2	-	1/10/11/13	0/1/1/1
1	PTR	B	527	1,2	-	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	-2.96	1.47	1.53
1	B	527	PTR	P-O3P	-2.30	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	527	PTR	CB-CA-C	-4.17	103.65	111.47
1	A	527	PTR	OH-CZ-CE2	-3.52	108.75	119.23
1	A	527	PTR	CB-CG-CD2	-3.10	114.74	120.91
1	A	527	PTR	O2P-P-OH	3.00	114.63	105.24
1	A	527	PTR	OH-CZ-CE1	2.92	127.91	119.23
1	B	527	PTR	O2P-P-OH	2.70	113.67	105.24
1	A	527	PTR	CD1-CE1-CZ	-2.69	116.44	119.73
1	A	527	PTR	CE2-CZ-CE1	2.05	123.34	120.18

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 carbohydrates 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	-	21,24,24	1.42	3 (14%)	28,36,36	2.66	11 (39%)
3	QUE	B	532	-	21,24,24	1.71	8 (38%)	28,36,36	3.03	12 (42%)

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	-	-	2/4/4/4	0/3/3/3
3	QUE	B	532	-	-	2/4/4/4	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	532	QUE	C14-C11	-3.12	1.41	1.46
3	B	532	QUE	C1-C2	2.71	1.43	1.37
3	A	1	QUE	C1-C2	2.42	1.43	1.37
3	B	532	QUE	O24-C17	2.35	1.41	1.36
3	B	532	QUE	C16-C17	2.28	1.43	1.39
3	B	532	QUE	O27-C10	2.13	1.42	1.35
3	B	532	QUE	C16-C15	2.12	1.42	1.38
3	A	1	QUE	O24-C17	2.11	1.40	1.36
3	A	1	QUE	O23-C18	2.10	1.40	1.36
3	B	532	QUE	O23-C18	2.09	1.40	1.36
3	B	532	QUE	C1-C6	2.02	1.42	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	532	QUE	C5-C6-C1	-7.70	114.72	120.94
3	A	1	QUE	C5-C6-C1	-7.10	115.21	120.94
3	B	532	QUE	C14-C19-C18	7.00	126.26	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	QUE	C14-C19-C18	6.67	125.99	120.68
3	B	532	QUE	C15-C14-C11	5.27	127.64	120.29
3	A	1	QUE	C15-C14-C11	4.87	127.08	120.29
3	B	532	QUE	C2-C3-C4	-4.71	112.35	117.82
3	A	1	QUE	C2-C1-C6	4.42	123.70	119.70
3	B	532	QUE	C2-C1-C6	3.77	123.11	119.70
3	B	532	QUE	C9-C3-C2	3.67	128.15	121.85
3	B	532	QUE	C9-C10-C11	-3.37	113.70	119.45
3	B	532	QUE	C19-C18-C17	-3.35	116.90	119.86
3	B	532	QUE	C19-C14-C11	-3.23	115.78	120.29
3	A	1	QUE	O12-C4-C3	-3.02	118.06	121.03
3	B	532	QUE	O12-C4-C3	-2.94	118.14	121.03
3	A	1	QUE	C19-C18-C17	-2.71	117.46	119.86
3	A	1	QUE	O23-C18-C17	2.62	125.44	118.45
3	B	532	QUE	O29-C6-C1	2.52	126.40	119.84
3	A	1	QUE	C2-C3-C4	-2.46	114.97	117.82
3	A	1	QUE	C15-C14-C19	-2.43	114.73	118.16
3	B	532	QUE	O23-C18-C17	2.40	124.85	118.45
3	A	1	QUE	O12-C4-C5	2.04	118.49	116.11
3	A	1	QUE	O24-C17-C18	2.03	123.87	118.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	QUE	C10-C11-C14-C15
3	A	1	QUE	C10-C11-C14-C19
3	B	532	QUE	C10-C11-C14-C15
3	B	532	QUE	C10-C11-C14-C19

There are no ring outliers.

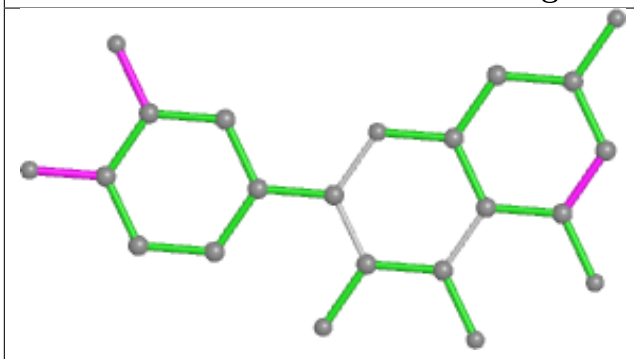
2 monomers are involved in 2 short contacts:

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

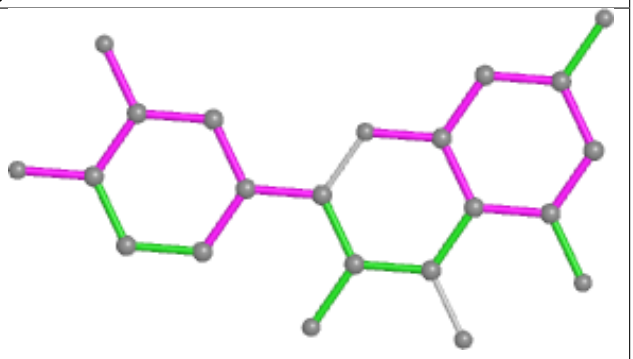
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

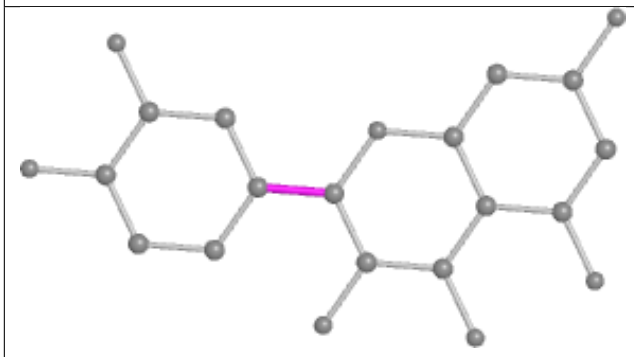
Ligand QUE A 1



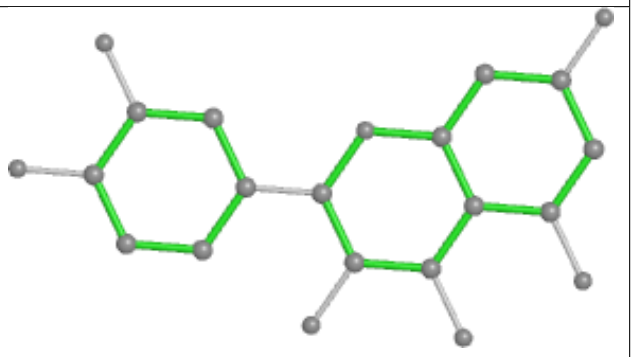
Bond lengths



Bond angles

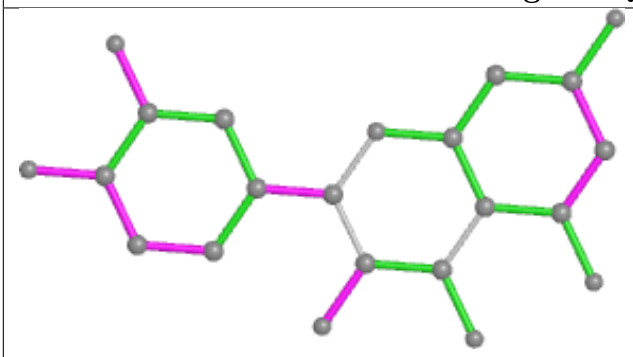


Torsions

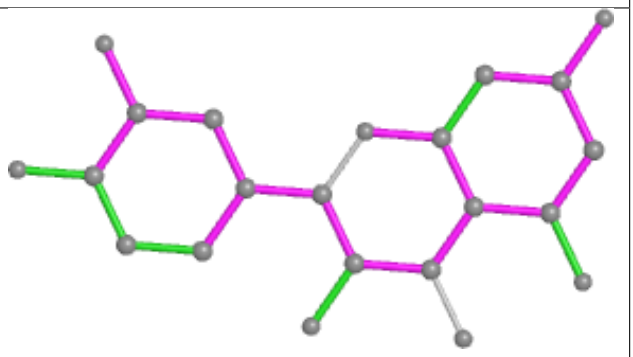


Rings

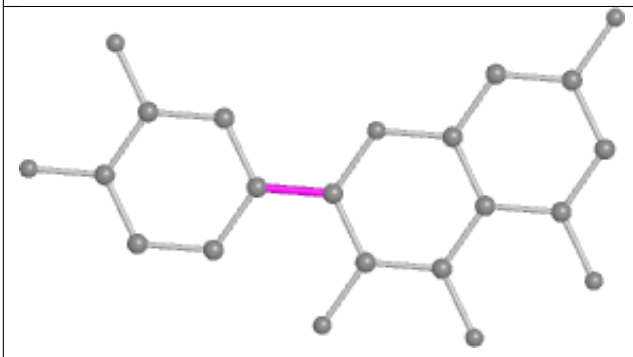
Ligand QUE B 532



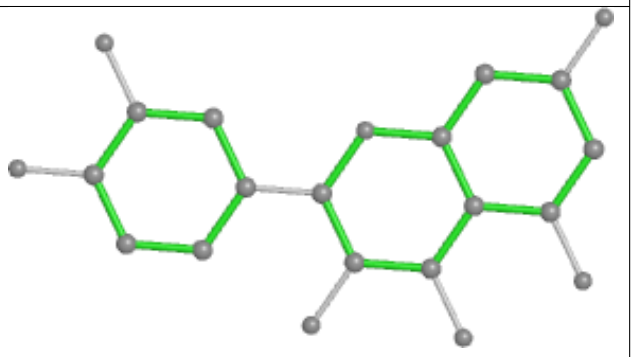
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	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.