Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:43 am BST

PDB ID	:	1H1R
Title	:	Structure of human Thr160-phospho CDK2/cyclin A complexed with the inhibitor NU6086
Authors	:	Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.
Deposited on	:	2002-07-21
Resolution	:	2.00 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:

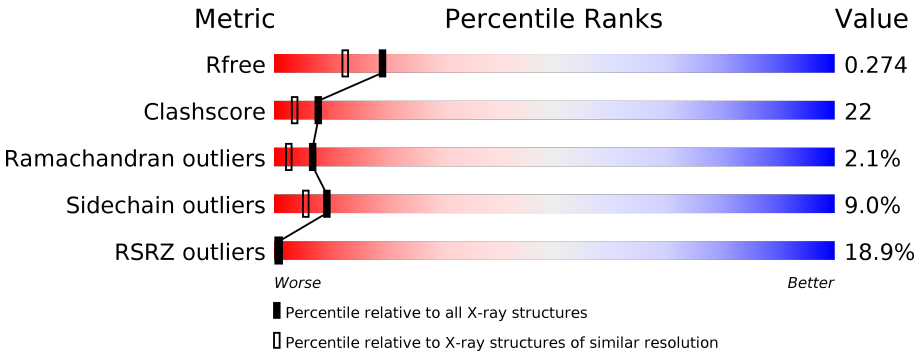
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	6% 64% 25% 6%
1	C	303	31% 48% 39% 8%
2	B	258	5% 75% 17% 5%
2	D	258	33% 45% 47% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9765 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.

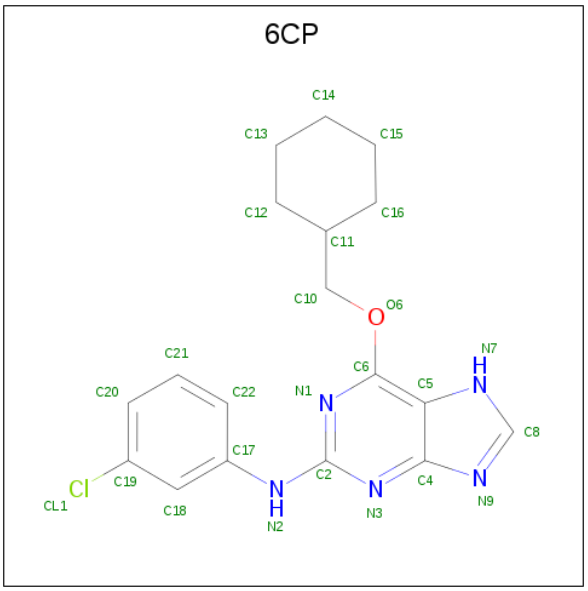
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 6-CYCLOHEXYLMETHOXY-2-(3'-CHLOROANILINO) PURINE (three-letter code: 6CP) (formula: $C_{18}H_{20}ClN_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	1
			50	36	2	10	2		
3	C	1	Total	C	Cl	N	O	0	1
			50	36	2	10	2		

- Molecule 4 is water.

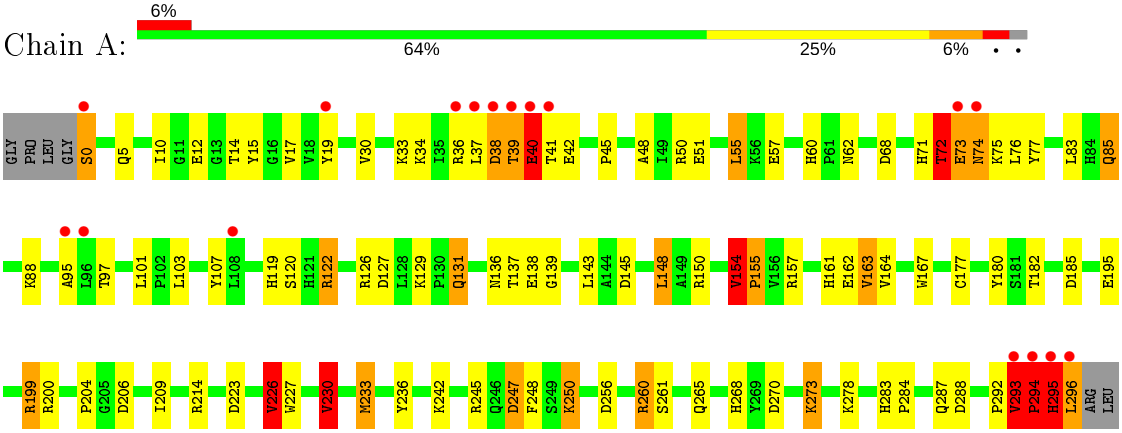
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		
4	B	229	Total	O	0	0
			229	229		
4	C	145	Total	O	0	0
			145	145		
4	D	83	Total	O	0	0
			83	83		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

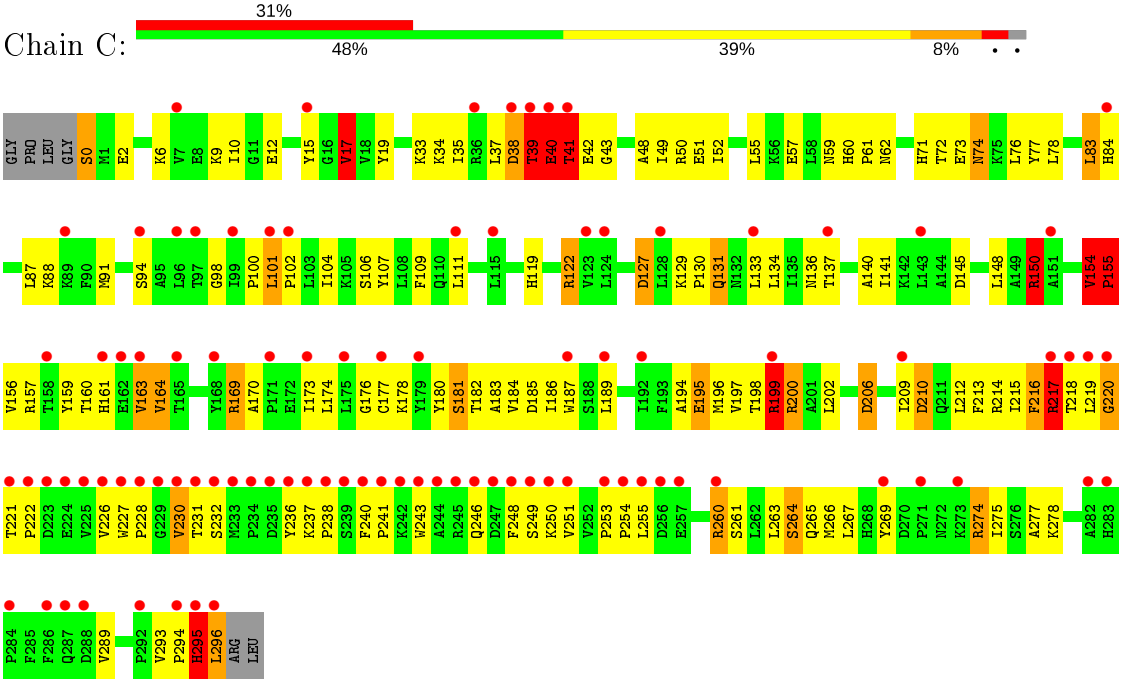
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A:



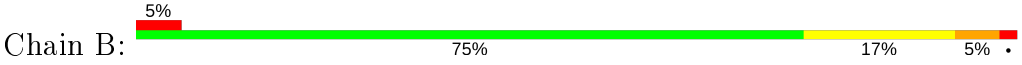
- Molecule 1: CELL DIVISION PROTEIN KINASE 2

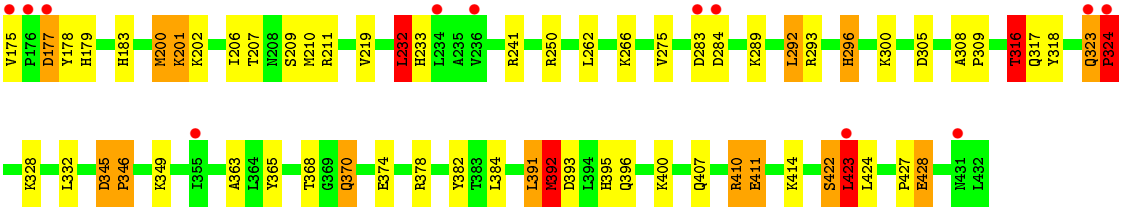
Chain C:



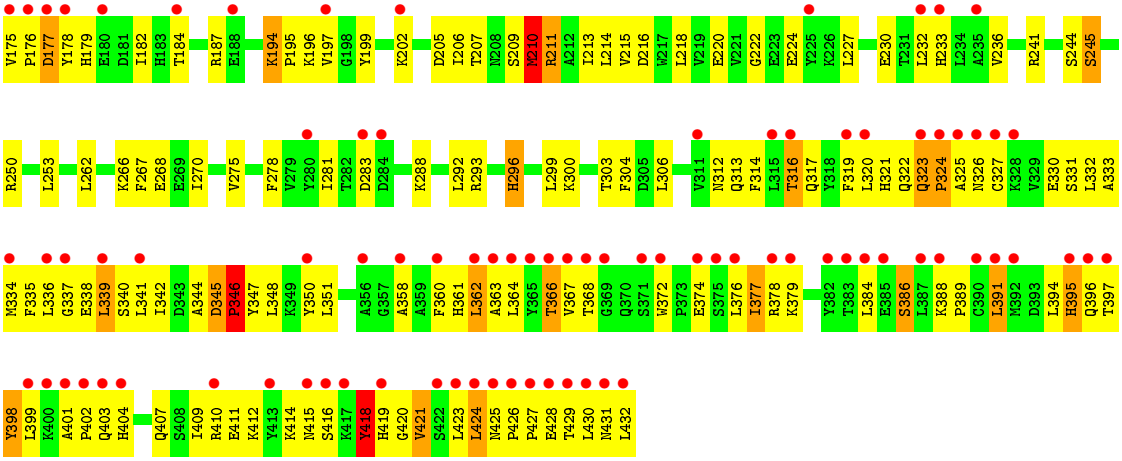
- Molecule 2: CYCLIN A2

Chain B:





- Molecule 2: CYCLIN A2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.11Å 134.95Å 148.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 32.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.00) 92.8 (32.20-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.235 , 0.294 0.225 , 0.274	Depositor DCC
R_{free} test set	4696 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 80.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9765	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 6CP

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	0.87	2/2438 (0.1%)	2.02	70/3308 (2.1%)
1	C	0.62	0/2438	1.71	43/3308 (1.3%)
2	B	0.80	0/2133	1.72	36/2897 (1.2%)
2	D	0.62	0/2133	1.61	30/2897 (1.0%)
All	All	0.74	2/9142 (0.0%)	1.78	179/12410 (1.4%)

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	4
1	C	0	2
2	B	0	5
2	D	0	4
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	SER	CA-CB	5.75	1.61	1.52
1	A	293	VAL	N-CA	5.40	1.57	1.46

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ARG	CD-NE-CZ	27.03	161.44	123.60
1	A	199	ARG	CD-NE-CZ	24.57	158.00	123.60
1	C	217	ARG	CD-NE-CZ	24.00	157.20	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	PRO	C-N-CA	22.15	177.06	121.70
1	A	295	HIS	N-CA-CB	18.07	143.12	110.60
1	A	199	ARG	NE-CZ-NH2	-17.67	111.47	120.30
1	A	250	LYS	CG-CD-CE	15.88	159.54	111.90
2	B	423	LEU	CB-CA-C	15.57	139.78	110.20
1	A	295	HIS	CA-CB-CG	14.08	137.54	113.60
1	A	245	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	A	295	HIS	C-N-CA	13.17	154.62	121.70
2	D	241	ARG	NE-CZ-NH2	-12.70	113.95	120.30
2	D	378	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	A	294	PRO	O-C-N	-12.23	103.13	122.70
1	A	293	VAL	CB-CA-C	12.18	134.54	111.40
2	D	378	ARG	CD-NE-CZ	11.91	140.28	123.60
2	B	177	ASP	CB-CG-OD1	11.90	129.01	118.30
2	D	296	HIS	CA-CB-CG	11.70	133.49	113.60
1	A	245	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	C	274	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	D	345	ASP	CA-C-O	-11.15	96.68	120.10
1	C	200	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	A	294	PRO	CA-C-N	10.30	139.86	117.20
1	A	293	VAL	N-CA-CB	-10.14	89.18	111.50
1	A	295	HIS	CB-CA-C	-10.07	90.26	110.40
2	D	324	PRO	CA-N-CD	-9.54	98.14	111.50
2	B	423	LEU	CB-CG-CD1	9.44	127.05	111.00
1	A	260	ARG	NE-CZ-NH1	9.39	124.99	120.30
2	B	324	PRO	CA-N-CD	-9.33	98.44	111.50
1	A	270	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	295	HIS	CA-C-O	9.28	139.58	120.10
1	C	274	ARG	CD-NE-CZ	9.08	136.31	123.60
1	C	154	VAL	CA-C-O	-9.04	101.12	120.10
1	A	126	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	293	VAL	CA-CB-CG1	8.84	124.16	110.90
2	B	241	ARG	NE-CZ-NH1	8.81	124.70	120.30
2	D	323	GLN	CA-C-O	-8.48	102.28	120.10
2	B	382	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	C	39	THR	C-N-CA	8.47	142.87	121.70
1	A	50	ARG	NE-CZ-NH2	-8.34	116.13	120.30
2	B	241	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	210	ASP	CB-CG-OD2	8.28	125.75	118.30
1	C	155	PRO	CA-N-CD	-8.02	100.27	111.50
1	C	217	ARG	CB-CG-CD	8.00	132.40	111.60
1	C	150	ARG	NE-CZ-NH2	-7.98	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	260	ARG	CD-NE-CZ	7.97	134.76	123.60
1	A	19	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	C	169	ARG	NE-CZ-NH2	-7.96	116.32	120.30
2	B	323	GLN	CA-C-O	-7.96	103.39	120.10
1	C	50	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	B	178	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	A	127	ASP	CB-CG-OD1	7.83	125.35	118.30
2	B	305	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	122	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	199	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	230	VAL	CB-CA-C	-7.67	96.82	111.40
1	C	122	ARG	CA-CB-CG	7.66	130.26	113.40
2	D	293	ARG	CD-NE-CZ	7.62	134.27	123.60
1	A	163	VAL	N-CA-CB	-7.56	94.86	111.50
2	B	392	MET	CG-SD-CE	7.40	112.04	100.20
1	A	122	ARG	CA-CB-CG	7.36	129.58	113.40
1	A	157	ARG	CD-NE-CZ	7.34	133.87	123.60
2	D	424	LEU	CA-CB-CG	7.23	131.94	115.30
1	C	199	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	C	50	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	D	216	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	157	ARG	CA-CB-CG	7.16	129.15	113.40
2	B	423	LEU	CA-CB-CG	7.15	131.74	115.30
2	B	378	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	393	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	295	HIS	N-CA-CB	7.12	123.42	110.60
2	B	318	TYR	CB-CG-CD1	7.11	125.27	121.00
2	D	241	ARG	NH1-CZ-NH2	7.10	127.21	119.40
1	A	155	PRO	CA-N-CD	-7.05	101.63	111.50
2	B	316	THR	N-CA-CB	-7.02	96.96	110.30
2	B	422	SER	C-N-CA	-6.98	104.25	121.70
2	B	345	ASP	CA-C-O	-6.96	105.49	120.10
1	C	206	ASP	CB-CG-OD1	-6.93	112.06	118.30
2	D	395	HIS	CA-CB-CG	6.90	125.34	113.60
1	C	40	GLU	CA-C-O	6.89	134.56	120.10
1	A	145	ASP	CB-CG-OD1	6.88	124.50	118.30
1	C	50	ARG	CD-NE-CZ	-6.67	114.25	123.60
1	A	57	GLU	OE1-CD-OE2	-6.67	115.30	123.30
2	D	346	PRO	CA-N-CD	-6.66	102.17	111.50
1	C	127	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	155	PRO	N-CA-CB	6.65	111.28	103.30
1	A	230	VAL	N-CA-CB	6.61	126.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	206	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	288	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	40	GLU	C-N-CA	6.54	138.06	121.70
1	A	145	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	39	THR	N-CA-CB	6.50	122.64	110.30
1	A	292	PRO	O-C-N	-6.48	112.33	122.70
1	C	206	ASP	OD1-CG-OD2	6.41	135.48	123.30
2	B	411	GLU	CB-CA-C	-6.39	97.62	110.40
2	D	199	TYR	CB-CG-CD1	6.38	124.83	121.00
1	C	57	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	C	40	GLU	CA-C-N	-6.32	103.29	117.20
1	C	41	THR	N-CA-C	-6.32	93.93	111.00
1	A	154	VAL	CA-C-O	-6.30	106.87	120.10
2	B	318	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	233	MET	CG-SD-CE	6.23	110.17	100.20
1	C	195	GLU	OE1-CD-OE2	-6.23	115.83	123.30
1	A	295	HIS	CA-C-N	-6.21	103.54	117.20
1	A	209	ILE	O-C-N	-6.20	112.78	122.70
1	A	36	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	51	GLU	OE1-CD-OE2	-6.13	115.94	123.30
2	B	201	LYS	CA-CB-CG	6.13	126.89	113.40
1	A	180	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	B	346	PRO	CA-N-CD	-6.09	102.97	111.50
1	A	85	GLN	N-CA-CB	-6.07	99.67	110.60
1	A	293	VAL	O-C-N	-6.04	109.61	121.10
1	C	17	VAL	CB-CA-C	-6.03	99.95	111.40
1	A	40	GLU	CA-C-O	5.98	132.66	120.10
1	A	143	LEU	CB-CG-CD1	5.94	121.10	111.00
2	D	220	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	C	216	PHE	CB-CG-CD1	5.93	124.95	120.80
1	C	157	ARG	CD-NE-CZ	5.92	131.89	123.60
2	D	210	MET	CA-CB-CG	5.88	123.30	113.30
1	C	200	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	40	GLU	N-CA-CB	5.88	121.19	110.60
2	B	349	LYS	CA-CB-CG	5.87	126.31	113.40
1	C	157	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	73	GLU	CA-CB-CG	5.83	126.22	113.40
1	C	199	ARG	NE-CZ-NH1	-5.83	117.39	120.30
2	B	370	GLN	CA-CB-CG	5.82	126.19	113.40
1	C	127	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	30	VAL	CA-CB-CG2	5.80	119.60	110.90
2	D	211	ARG	NE-CZ-NH2	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	122	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	D	350	TYR	CB-CG-CD1	5.72	124.43	121.00
2	D	250	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	55	LEU	CB-CG-CD1	5.66	120.62	111.00
1	A	122	ARG	CD-NE-CZ	5.64	131.49	123.60
2	B	410	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	B	324	PRO	N-CD-CG	5.59	111.58	103.20
2	B	232	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	68	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	214	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	B	346	PRO	N-CA-CB	5.51	109.91	103.30
1	A	19	TYR	CB-CA-C	-5.50	99.41	110.40
2	D	177	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	120	SER	CA-CB-OG	-5.45	96.49	111.20
1	A	157	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	236	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	D	205	ASP	CB-CG-OD2	5.41	123.17	118.30
2	D	199	TYR	CA-CB-CG	5.40	123.66	113.40
2	B	423	LEU	O-C-N	-5.40	114.06	122.70
1	A	247	ASP	N-CA-CB	-5.37	100.93	110.60
2	D	224	GLU	CA-CB-CG	5.36	125.19	113.40
1	A	157	ARG	CB-CA-C	-5.35	99.69	110.40
1	A	256	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	150	ARG	NH1-CZ-NH2	5.35	125.29	119.40
2	D	245	SER	CB-CA-C	-5.35	99.94	110.10
2	D	350	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	14	THR	CA-CB-CG2	-5.32	104.95	112.40
2	D	296	HIS	N-CA-CB	-5.32	101.03	110.60
1	A	250	LYS	CB-CG-CD	5.29	125.35	111.60
1	C	155	PRO	N-CD-CG	5.27	111.10	103.20
1	C	216	PHE	CB-CG-CD2	-5.25	117.12	120.80
2	D	253	LEU	CA-C-O	5.23	131.08	120.10
2	B	423	LEU	CB-CG-CD2	-5.21	102.15	111.00
2	B	200	MET	CG-SD-CE	5.20	108.53	100.20
1	A	39	THR	N-CA-CB	5.20	120.18	110.30
2	B	232	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	226	VAL	CG1-CB-CG2	-5.18	102.61	110.90
2	D	418	TYR	CA-CB-CG	5.18	123.24	113.40
1	C	150	ARG	CA-CB-CG	5.17	124.77	113.40
1	A	72	THR	N-CA-CB	-5.16	100.50	110.30
2	B	365	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	162	GLU	O-C-N	5.13	130.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	267	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	B	422	SER	N-CA-CB	5.11	118.16	110.50
1	A	233	MET	CA-CB-CG	-5.11	104.62	113.30
1	A	288	ASP	CB-CG-OD2	-5.05	113.76	118.30
2	D	283	ASP	N-CA-CB	5.04	119.67	110.60
2	B	296	HIS	N-CA-CB	-5.04	101.53	110.60
2	B	391	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	230	VAL	CA-CB-CG1	5.00	118.40	110.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	154	VAL	Mainchain,Peptide
1	A	293	VAL	Mainchain
2	B	323	GLN	Mainchain,Peptide
2	B	345	ASP	Mainchain,Peptide
2	B	423	LEU	Mainchain
1	C	154	VAL	Mainchain,Peptide
2	D	323	GLN	Mainchain,Peptide
2	D	345	ASP	Mainchain,Peptide

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	2388	0	2428	83	0
1	C	2388	0	2429	153	0
2	B	2083	0	2107	59	0
2	D	2083	0	2107	110	0
3	A	50	0	39	1	0
3	C	50	0	39	8	0
4	A	266	0	0	16	0
4	B	229	0	0	12	0
4	C	145	0	0	46	0
4	D	83	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9765	0	9149	392	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 22.

All (392) 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:230:VAL:HA	1:A:233:MET:HE3	1.35	1.04
2:B:423:LEU:HB2	4:B:2222:HOH:O	1.63	0.98
1:A:177:CYS:HB2	4:A:2152:HOH:O	1.68	0.90
1:A:41:THR:HG22	1:A:42:GLU:H	1.39	0.88
2:B:177:ASP:HB2	4:B:2048:HOH:O	1.74	0.86
2:D:376:LEU:HD23	2:D:379:LYS:HD3	1.58	0.85
1:C:130:PRO:HA	4:C:2084:HOH:O	1.75	0.85
1:A:60:HIS:HD2	1:A:62:ASN:H	1.25	0.84
2:B:422:SER:OG	2:B:423:LEU:HD12	1.78	0.83
3:C:1298[B]:6CP:H18	3:C:1298[B]:6CP:N1	1.94	0.82
3:C:1298[A]:6CP:N1	3:C:1298[A]:6CP:H18	1.94	0.82
1:C:218:THR:HG22	1:C:219:LEU:HG	1.60	0.82
1:A:72:THR:HG22	1:A:75:LYS:H	1.43	0.82
1:A:41:THR:HA	4:A:2043:HOH:O	1.78	0.82
1:C:183:ALA:HB1	1:C:274:ARG:HH11	1.44	0.81
1:A:230:VAL:HA	1:A:233:MET:CE	2.12	0.80
2:D:275:VAL:HG11	2:D:292:LEU:HD21	1.64	0.80
1:C:277:ALA:HB3	4:D:2009:HOH:O	1.83	0.79
1:A:230:VAL:CA	1:A:233:MET:HE3	2.11	0.79
1:A:60:HIS:CD2	1:A:62:ASN:H	2.01	0.79
1:A:161:HIS:HD2	4:A:2136:HOH:O	1.65	0.79
1:C:83:LEU:HD13	1:C:134:LEU:HB2	1.65	0.78
1:C:174:LEU:HB3	1:C:212:LEU:HD21	1.64	0.78
2:D:194:LYS:HD3	2:D:351:LEU:HD23	1.66	0.78
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.66	0.77
2:B:414:LYS:HG2	2:B:423:LEU:HD13	1.66	0.77
2:B:414:LYS:HG2	2:B:423:LEU:CD1	2.15	0.77
1:C:156:VAL:HG11	1:C:181:SER:HB2	1.67	0.76
2:B:296:HIS:NE2	2:B:300:LYS:HE2	1.99	0.76
1:C:243:TRP:HA	4:C:2124:HOH:O	1.83	0.76
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.69	0.75
2:B:328:LYS:NZ	2:B:424:LEU:HD21	2.02	0.75
2:B:316:THR:HG21	4:B:2023:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:VAL:N	2:D:176:PRO:CD	2.50	0.74
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.22	0.74
1:C:37:LEU:O	1:C:38:ASP:HB2	1.86	0.73
1:C:227:TRP:O	1:C:230:VAL:HG22	1.88	0.73
1:A:139:GLY:CA	1:A:293:VAL:HA	2.18	0.73
1:C:0:SER:O	4:C:2002:HOH:O	2.07	0.73
2:B:423:LEU:CB	4:B:2222:HOH:O	2.28	0.72
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.71	0.72
1:C:177:CYS:HB2	4:C:2102:HOH:O	1.90	0.72
1:C:263:LEU:HD12	4:C:2134:HOH:O	1.89	0.72
1:C:218:THR:HA	1:C:246:GLN:HG3	1.70	0.72
2:D:322:GLN:NE2	2:D:326:ASN:H	1.88	0.71
1:A:88:LYS:HD3	1:A:131:GLN:HE22	1.56	0.71
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.73	0.71
1:A:39:THR:HG22	1:A:40:GLU:H	1.56	0.70
1:C:221:THR:HB	4:C:2111:HOH:O	1.90	0.70
1:C:41:THR:HB	4:C:2046:HOH:O	1.91	0.70
2:B:328:LYS:HZ1	2:B:424:LEU:HD21	1.57	0.70
1:C:0:SER:HA	4:C:2002:HOH:O	1.91	0.70
2:D:322:GLN:HE21	2:D:325:ALA:HA	1.55	0.69
1:C:181:SER:OG	1:C:182:THR:N	2.26	0.69
1:C:198:THR:O	1:C:199:ARG:HB2	1.91	0.69
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.75	0.69
1:C:267:LEU:HG	4:C:2134:HOH:O	1.92	0.69
1:C:238:PRO:HD3	4:C:2118:HOH:O	1.92	0.68
2:D:196:LYS:HG2	2:D:244:SER:HB3	1.75	0.68
2:D:206:ILE:HG22	2:D:210:MET:CE	2.23	0.68
1:A:138:GLU:HG2	4:A:2116:HOH:O	1.94	0.68
3:C:1298[A]:6CP:C18	3:C:1298[A]:6CP:N1	2.52	0.68
3:C:1298[B]:6CP:C18	3:C:1298[B]:6CP:N1	2.52	0.68
1:C:60:HIS:HD2	1:C:62:ASN:H	1.41	0.68
1:C:212:LEU:HD22	4:C:2108:HOH:O	1.95	0.67
2:D:358:ALA:HB1	2:D:391:LEU:HD13	1.76	0.67
1:C:164:VAL:HG13	4:C:2082:HOH:O	1.95	0.67
2:D:418:TYR:HB2	4:D:2071:HOH:O	1.93	0.67
1:A:74:ASN:ND2	1:A:74:ASN:H	1.92	0.67
1:C:42:GLU:HG3	4:C:2048:HOH:O	1.94	0.67
2:D:388:LYS:HG3	2:D:432:LEU:HD13	1.76	0.66
1:C:187:TRP:HB2	4:C:2139:HOH:O	1.95	0.66
1:C:155:PRO:HD3	2:D:320:LEU:HD21	1.78	0.66
1:A:137:THR:O	1:A:293:VAL:HG13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD12	4:C:2084:HOH:O	1.94	0.65
1:C:87:LEU:HD23	4:C:2084:HOH:O	1.94	0.65
1:A:154:VAL:O	2:B:316:THR:HG23	1.96	0.65
2:D:321:HIS:ND1	2:D:376:LEU:HG	2.12	0.64
2:B:289:LYS:HG2	2:B:293:ARG:HH21	1.61	0.64
1:C:137:THR:HG22	1:C:296:LEU:CD1	2.28	0.64
2:D:429:THR:HA	4:D:2079:HOH:O	1.96	0.64
1:A:293:VAL:HG12	1:A:294:PRO:HD2	1.80	0.64
1:C:127:ASP:HA	4:C:2082:HOH:O	1.98	0.63
1:A:34:LYS:HE3	1:A:75:LYS:HD3	1.80	0.63
1:C:60:HIS:CD2	1:C:62:ASN:H	2.17	0.62
2:D:376:LEU:HA	2:D:379:LYS:HB3	1.81	0.62
1:A:248:PHE:HB2	4:A:2223:HOH:O	1.98	0.62
1:C:6:LYS:HG3	4:C:2007:HOH:O	1.99	0.62
2:D:430:LEU:HB2	4:D:2083:HOH:O	1.99	0.62
1:C:209:ILE:HD11	1:C:213:PHE:CZ	2.35	0.62
1:C:34:LYS:HE3	1:C:77:TYR:OH	1.99	0.62
2:D:176:PRO:HA	2:D:179:HIS:CD2	2.34	0.62
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.82	0.61
2:D:321:HIS:HB2	2:D:376:LEU:HD11	1.80	0.61
1:C:195:GLU:HB2	4:C:2104:HOH:O	2.01	0.61
1:C:17:VAL:HG22	4:C:2011:HOH:O	2.00	0.61
1:C:154:VAL:O	2:D:316:THR:HG23	1.99	0.61
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.01	0.61
1:C:129:LYS:HG3	1:C:131:GLN:HG2	1.82	0.60
2:B:423:LEU:HB3	4:B:2220:HOH:O	2.01	0.60
1:A:34:LYS:HE3	1:A:75:LYS:CD	2.32	0.60
1:C:130:PRO:HG3	4:C:2105:HOH:O	2.01	0.60
2:D:425:ASN:HA	4:D:2073:HOH:O	2.00	0.60
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.31	0.60
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.84	0.60
2:D:336:LEU:HA	2:D:339:LEU:HD12	1.83	0.60
1:A:250:LYS:HD3	4:A:2090:HOH:O	2.01	0.59
1:C:84:HIS:CG	1:C:296:LEU:HD13	2.37	0.59
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.37	0.59
1:C:10:ILE:HG21	3:C:1298[A]:6CP:H101	1.84	0.59
1:C:10:ILE:HG21	3:C:1298[B]:6CP:H101	1.84	0.59
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.84	0.59
2:D:175:VAL:N	2:D:176:PRO:HD2	2.18	0.59
1:C:35:ILE:HA	4:C:2017:HOH:O	2.03	0.59
1:C:248:PHE:HA	1:C:251:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:MET:HA	2:B:392:MET:CE	2.34	0.58
2:D:278:PHE:O	2:D:281:ILE:HG12	2.03	0.58
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.39	0.58
2:D:427:PRO:HA	4:D:2076:HOH:O	2.03	0.58
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.84	0.58
2:D:399:LEU:HD23	2:D:426:PRO:HG2	1.86	0.58
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.57
1:C:183:ALA:HB1	1:C:274:ARG:NH1	2.16	0.57
1:C:261:SER:O	1:C:265:GLN:HG3	2.05	0.57
1:C:88:LYS:HD3	1:C:131:GLN:NE2	2.20	0.57
2:B:423:LEU:HD13	4:B:2222:HOH:O	2.05	0.57
1:A:41:THR:HG22	1:A:42:GLU:N	2.16	0.56
1:C:84:HIS:CD2	1:C:296:LEU:HD22	2.41	0.56
2:D:196:LYS:CG	2:D:244:SER:HB3	2.35	0.56
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.89	0.56
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.36	0.56
2:D:421:VAL:HA	2:D:424:LEU:HG	1.88	0.56
1:A:107:TYR:OH	1:A:294:PRO:HB3	2.06	0.56
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.87	0.55
1:C:184:VAL:HB	4:C:2103:HOH:O	2.05	0.55
1:C:197:VAL:HG21	1:C:255:LEU:HD13	1.89	0.55
1:C:156:VAL:HB	1:C:159:TYR:CE2	2.42	0.55
2:D:288:LYS:O	2:D:292:LEU:HD23	2.07	0.55
1:C:91:MET:HE2	1:C:196:MET:HG3	1.89	0.55
1:C:228:PRO:HA	4:C:2113:HOH:O	2.07	0.55
1:A:74:ASN:ND2	1:A:74:ASN:N	2.55	0.54
2:D:321:HIS:CB	2:D:376:LEU:HD11	2.37	0.54
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.37	0.54
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.42	0.54
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.89	0.54
1:A:39:THR:HG21	2:B:289:LYS:HE3	1.90	0.54
1:A:5:GLN:NE2	4:A:2005:HOH:O	2.40	0.54
1:A:227:TRP:O	1:A:230:VAL:HG22	2.07	0.54
1:A:88:LYS:HD3	1:A:131:GLN:NE2	2.20	0.54
1:C:215:ILE:HG23	4:C:2109:HOH:O	2.07	0.54
1:C:51:GLU:O	1:C:55:LEU:HB2	2.07	0.54
1:A:247:ASP:HB3	1:A:250:LYS:HG3	1.90	0.54
1:C:107:TYR:O	1:C:111:LEU:HG	2.08	0.54
1:A:74:ASN:N	1:A:74:ASN:HD22	2.05	0.54
2:B:207:THR:OG1	2:B:210:MET:HG3	2.08	0.54
2:B:392:MET:HE2	4:B:2197:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:MET:CE	1:C:196:MET:HG3	2.38	0.53
1:A:161:HIS:CD2	4:A:2136:HOH:O	2.50	0.53
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.53
2:D:209:SER:O	2:D:213:ILE:HG13	2.08	0.53
1:C:219:LEU:HD13	4:C:2135:HOH:O	2.08	0.53
1:C:220:GLY:HA2	1:C:243:TRP:O	2.07	0.53
1:C:181:SER:O	1:C:184:VAL:HG22	2.09	0.53
2:D:312:ASN:HB3	4:D:2055:HOH:O	2.07	0.53
1:A:139:GLY:HA3	1:A:293:VAL:HA	1.90	0.53
2:D:386:SER:O	2:D:389:PRO:HD2	2.08	0.53
1:A:230:VAL:CG1	1:A:233:MET:HE3	2.38	0.53
1:C:84:HIS:NE2	1:C:296:LEU:HB3	2.23	0.53
2:D:366:THR:OG1	2:D:427:PRO:HD3	2.09	0.53
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.44	0.53
1:C:137:THR:O	1:C:293:VAL:HG13	2.08	0.53
2:B:206:ILE:HA	2:B:210:MET:SD	2.49	0.52
2:D:322:GLN:HE22	2:D:326:ASN:H	1.54	0.52
2:B:183:HIS:HD2	4:B:2058:HOH:O	1.92	0.52
1:C:0:SER:CA	4:C:2002:HOH:O	2.54	0.52
1:A:136:ASN:O	1:A:294:PRO:HG3	2.09	0.52
2:D:211:ARG:O	2:D:215:VAL:HG23	2.08	0.52
1:C:238:PRO:HB2	4:C:2120:HOH:O	2.10	0.52
1:C:289:VAL:HA	4:C:2143:HOH:O	2.07	0.52
2:D:313:GLN:O	2:D:316:THR:HG22	2.09	0.52
2:D:366:THR:HG22	2:D:367:VAL:HG23	1.92	0.52
1:A:119:HIS:CD2	1:A:182:THR:HB	2.44	0.52
2:B:233:HIS:HE1	4:B:2159:HOH:O	1.92	0.52
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.92	0.52
2:D:270:ILE:HG13	4:D:2036:HOH:O	2.10	0.52
1:C:164:VAL:HA	4:C:2082:HOH:O	2.09	0.52
1:C:249:SER:HA	1:C:260:ARG:HD3	1.91	0.52
1:A:15:TYR:OH	1:A:48:ALA:HA	2.10	0.51
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.91	0.51
1:A:37:LEU:O	1:A:38:ASP:HB2	2.11	0.51
2:B:201:LYS:HD3	2:B:201:LYS:O	2.10	0.51
2:D:340:SER:HA	2:D:347:TYR:CD2	2.45	0.51
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.41	0.51
2:B:423:LEU:CD1	4:B:2222:HOH:O	2.58	0.51
1:C:83:LEU:HD13	1:C:134:LEU:CB	2.39	0.51
1:C:260:ARG:O	1:C:264:SER:OG	2.24	0.51
1:A:119:HIS:HD2	4:B:2049:HOH:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:NE2	1:C:176:GLY:HA2	2.26	0.51
1:C:183:ALA:CB	1:C:274:ARG:HH11	2.18	0.51
2:D:327:CYS:HB2	2:D:419:HIS:NE2	2.25	0.51
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.11	0.50
1:A:242:LYS:HB2	4:A:2209:HOH:O	2.11	0.50
2:D:360:PHE:O	2:D:364:LEU:HB2	2.11	0.50
2:D:399:LEU:CD2	2:D:426:PRO:HG2	2.42	0.50
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.46	0.50
1:C:101:LEU:N	1:C:102:PRO:HD2	2.27	0.50
1:C:219:LEU:HD12	4:C:2109:HOH:O	2.11	0.50
2:B:210:MET:CE	2:B:250:ARG:HB2	2.41	0.50
1:C:217:ARG:HG3	1:C:243:TRP:CD1	2.47	0.50
1:C:216:PHE:CE1	1:C:222:PRO:HD3	2.47	0.49
1:A:195:GLU:O	1:A:199:ARG:HA	2.11	0.49
1:C:231:THR:HA	1:C:236:TYR:CD1	2.47	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.47	0.49
1:A:74:ASN:H	1:A:74:ASN:HD22	1.60	0.49
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.47	0.49
1:A:39:THR:HG21	2:B:289:LYS:CE	2.42	0.49
2:B:392:MET:HA	2:B:392:MET:HE3	1.95	0.49
1:C:186:ILE:HG13	1:C:275:ILE:O	2.12	0.49
1:C:35:ILE:HB	1:C:76:LEU:HB3	1.94	0.49
2:D:430:LEU:O	2:D:431:ASN:HB2	2.13	0.49
1:A:60:HIS:HE1	4:A:2042:HOH:O	1.96	0.49
2:B:423:LEU:CG	4:B:2222:HOH:O	2.58	0.49
1:C:71:HIS:NE2	2:D:296:HIS:ND1	2.61	0.48
1:A:284:PRO:O	1:A:287:GLN:HG2	2.14	0.48
1:C:33:LYS:NZ	1:C:51:GLU:OE1	2.44	0.48
2:D:303:THR:O	2:D:304:PHE:HB2	2.13	0.48
2:B:395:HIS:HE1	2:B:427:PRO:O	1.96	0.48
1:C:217:ARG:HG3	1:C:243:TRP:CE2	2.48	0.48
1:C:129:LYS:HB3	4:C:2081:HOH:O	2.12	0.48
1:C:194:ALA:CB	1:C:202:LEU:HD22	2.43	0.48
1:C:220:GLY:O	1:C:221:THR:C	2.49	0.48
1:C:74:ASN:H	1:C:74:ASN:ND2	2.11	0.48
2:D:374:GLU:HA	2:D:377:ILE:CD1	2.44	0.48
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.41	0.48
2:D:407:GLN:O	2:D:411:GLU:HG2	2.13	0.48
1:A:139:GLY:HA2	1:A:293:VAL:HA	1.92	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.48
1:A:223:ASP:H	1:A:226:VAL:CG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LYS:CG	2:B:293:ARG:HH21	2.26	0.48
1:C:186:ILE:HD12	4:C:2141:HOH:O	2.13	0.48
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.97	0.48
2:B:211:ARG:HH11	2:B:211:ARG:HG2	1.79	0.48
2:D:362:LEU:HD21	2:D:395:HIS:HB2	1.96	0.48
1:A:97:THR:HG22	1:A:97:THR:O	2.14	0.48
1:C:39:THR:HG22	1:C:40:GLU:N	2.29	0.47
1:A:148:LEU:HD12	4:A:2119:HOH:O	2.14	0.47
1:C:150:ARG:NH2	1:C:160:TPO:O2P	2.47	0.47
1:A:85:GLN:OE1	1:A:296:LEU:HD22	2.13	0.47
2:B:211:ARG:NH1	2:B:211:ARG:HG2	2.29	0.47
2:D:332:LEU:HD12	2:D:335:PHE:CD2	2.50	0.47
2:D:332:LEU:HG	2:D:332:LEU:O	2.13	0.47
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.83	0.47
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.47
1:C:88:LYS:HD3	1:C:131:GLN:HE22	1.79	0.47
2:D:207:THR:OG1	2:D:210:MET:HG3	2.14	0.47
2:D:366:THR:HG22	2:D:367:VAL:N	2.29	0.47
1:C:174:LEU:HD13	1:C:212:LEU:HD23	1.97	0.47
1:C:212:LEU:HB3	4:C:2108:HOH:O	2.15	0.47
2:D:336:LEU:HA	2:D:339:LEU:CD1	2.45	0.47
1:C:150:ARG:HH21	1:C:160:TPO:P	2.37	0.47
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.49	0.47
2:D:347:TYR:OH	2:D:394:LEU:HA	2.15	0.47
2:D:414:LYS:HG2	2:D:423:LEU:HG	1.97	0.47
1:A:131:GLN:H	1:A:131:GLN:CD	2.19	0.46
2:B:414:LYS:HG2	2:B:423:LEU:HD11	1.97	0.46
1:C:194:ALA:HB3	1:C:202:LEU:HD22	1.97	0.46
1:A:72:THR:O	2:B:296:HIS:HE1	1.99	0.46
2:D:230:GLU:HA	4:D:2055:HOH:O	2.15	0.46
2:D:296:HIS:NE2	2:D:300:LYS:HE2	2.31	0.46
1:A:137:THR:O	1:A:293:VAL:CG1	2.63	0.46
1:C:231:THR:HA	1:C:236:TYR:CE1	2.51	0.46
1:C:100:PRO:O	1:C:104:ILE:HG13	2.16	0.46
1:C:17:VAL:HB	1:C:19:TYR:CE1	2.51	0.46
1:C:15:TYR:OH	1:C:48:ALA:HA	2.16	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46
2:D:232:LEU:O	2:D:236:VAL:HG23	2.16	0.46
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.51	0.46
1:C:156:VAL:HG21	1:C:180:TYR:O	2.16	0.45
1:C:98:GLY:HA2	1:C:199:ARG:NE	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.80	0.45
1:C:227:TRP:HA	1:C:228:PRO:HD2	1.63	0.45
2:D:319:PHE:CZ	2:D:333:ALA:HB3	2.52	0.45
1:C:266:MET:HG2	4:C:2141:HOH:O	2.16	0.45
2:D:361:HIS:CD2	2:D:384:LEU:HD11	2.51	0.45
2:D:342:ILE:HG21	2:D:404:HIS:CE1	2.51	0.45
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.98	0.45
1:C:184:VAL:HA	4:C:2139:HOH:O	2.16	0.45
2:B:283:ASP:O	2:B:284:ASP:HB2	2.15	0.45
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.20	0.45
1:C:169:ARG:HG2	1:C:173:ILE:HB	1.97	0.45
2:D:334:MET:O	2:D:335:PHE:C	2.55	0.45
2:D:396:GLN:O	2:D:399:LEU:N	2.50	0.45
2:D:409:ILE:O	2:D:412:LYS:HB3	2.15	0.45
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.45
2:D:395:HIS:CD2	2:D:430:LEU:HG	2.52	0.45
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.32	0.45
2:D:402:PRO:HB2	2:D:403:GLN:NE2	2.32	0.45
1:C:174:LEU:CB	1:C:212:LEU:HD21	2.42	0.45
1:A:103:LEU:HD13	1:A:293:VAL:O	2.17	0.44
1:C:274:ARG:NH1	4:C:2139:HOH:O	2.49	0.44
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.44
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.99	0.44
1:A:230:VAL:CG1	1:A:233:MET:CE	2.95	0.44
1:A:37:LEU:O	1:A:38:ASP:CB	2.65	0.44
2:D:404:HIS:O	2:D:407:GLN:NE2	2.43	0.44
1:C:236:TYR:HD2	4:C:2115:HOH:O	2.00	0.44
1:A:230:VAL:HG13	1:A:233:MET:CE	2.47	0.44
1:A:260:ARG:HD3	4:A:2230:HOH:O	2.16	0.44
2:B:296:HIS:NE2	2:B:300:LYS:CE	2.77	0.44
1:C:106:SER:O	1:C:109:PHE:N	2.51	0.44
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.86	0.44
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.83	0.44
2:D:332:LEU:CD2	2:D:363:ALA:HA	2.44	0.44
1:A:39:THR:HG22	2:B:292:LEU:HD23	1.99	0.44
1:C:111:LEU:HD21	1:C:141:ILE:HD13	2.00	0.44
2:D:210:MET:HE2	2:D:210:MET:HB2	1.84	0.44
1:A:268:HIS:CD2	4:A:2192:HOH:O	2.70	0.43
1:A:138:GLU:CG	4:A:2116:HOH:O	2.58	0.43
2:B:289:LYS:HG3	2:B:293:ARG:HE	1.83	0.43
1:C:295:HIS:C	1:C:295:HIS:ND1	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:HIS:HB2	4:D:2055:HOH:O	2.18	0.43
2:D:178:TYR:HB3	2:D:182:ILE:HG13	2.00	0.43
2:D:275:VAL:HG23	4:D:2040:HOH:O	2.18	0.43
1:C:88:LYS:CD	1:C:131:GLN:HE22	2.32	0.43
1:A:154:VAL:O	2:B:316:THR:CG2	2.65	0.43
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.88	0.43
2:D:184:THR:O	2:D:187:ARG:HB2	2.19	0.43
2:D:206:ILE:HG21	2:D:206:ILE:HD13	1.77	0.43
2:D:361:HIS:CE1	2:D:384:LEU:HD21	2.54	0.43
2:D:398:TYR:HD1	2:D:398:TYR:O	2.01	0.43
1:C:109:PHE:HD2	4:C:2038:HOH:O	2.01	0.43
1:C:10:ILE:CG2	3:C:1298[B]:6CP:H101	2.47	0.43
1:C:10:ILE:CG2	3:C:1298[A]:6CP:H101	2.47	0.43
1:C:129:LYS:O	1:C:133:LEU:HG	2.19	0.43
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.01	0.43
1:A:39:THR:HG21	2:B:289:LYS:HD2	2.01	0.42
2:B:275:VAL:HG11	2:B:292:LEU:HD13	2.00	0.42
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.87	0.42
4:C:2044:HOH:O	2:D:292:LEU:HD23	2.19	0.42
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.49	0.42
1:A:17:VAL:O	1:A:33:LYS:HA	2.19	0.42
1:A:39:THR:CG2	2:B:292:LEU:HD23	2.50	0.42
2:D:214:LEU:O	2:D:218:LEU:HG	2.19	0.42
1:C:170:ALA:HB2	4:C:2139:HOH:O	2.18	0.42
2:D:299:LEU:HD13	2:D:304:PHE:CE1	2.55	0.42
2:B:368:THR:CB	2:B:370:GLN:HE21	2.33	0.42
1:C:198:THR:O	1:C:199:ARG:CB	2.60	0.42
1:C:199:ARG:HG3	4:C:2106:HOH:O	2.19	0.42
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.55	0.42
1:C:43:GLY:HA3	2:D:292:LEU:HD12	2.01	0.42
2:D:314:PHE:HA	2:D:317:GLN:HG3	2.02	0.42
1:A:227:TRP:HB3	1:A:230:VAL:HG22	2.00	0.42
1:A:40:GLU:H	2:B:292:LEU:HD23	1.84	0.42
2:D:332:LEU:CD2	2:D:366:THR:HG21	2.49	0.42
2:D:332:LEU:HB2	2:D:421:VAL:HB	2.02	0.42
2:D:175:VAL:O	2:D:175:VAL:HG12	2.20	0.42
2:D:175:VAL:N	2:D:176:PRO:HD3	2.33	0.42
2:D:409:ILE:O	2:D:410:ARG:C	2.58	0.42
1:A:10:ILE:HD13	3:A:1298[A]:6CP:C18	2.50	0.42
1:C:217:ARG:HD3	1:C:243:TRP:NE1	2.35	0.41
2:D:361:HIS:HD2	2:D:391:LEU:HG	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:40:GLU:C	2.58	0.41
4:A:2158:HOH:O	2:B:175:VAL:HG12	2.20	0.41
1:C:101:LEU:HB3	1:C:102:PRO:HD3	2.01	0.41
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.55	0.41
1:C:39:THR:HG22	4:C:2044:HOH:O	2.21	0.41
1:C:38:ASP:HA	4:C:2041:HOH:O	2.21	0.41
1:C:215:ILE:HG12	4:C:2109:HOH:O	2.19	0.41
1:C:237:LYS:HA	1:C:238:PRO:HD3	1.93	0.41
1:C:177:CYS:SG	1:C:178:LYS:N	2.94	0.41
1:C:209:ILE:HG23	1:C:210:ASP:N	2.35	0.41
2:D:210:MET:O	2:D:213:ILE:HB	2.21	0.41
2:B:428:GLU:HG2	2:B:428:GLU:H	1.56	0.41
2:D:206:ILE:HA	2:D:210:MET:CE	2.51	0.41
1:A:261:SER:O	1:A:265:GLN:HG3	2.21	0.41
1:C:156:VAL:HB	1:C:159:TYR:HE2	1.83	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.92	0.41
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.47	0.40
2:B:275:VAL:HG11	2:B:292:LEU:CD1	2.51	0.40
2:B:410:ARG:HH21	2:B:410:ARG:HD3	1.60	0.40
2:B:424:LEU:HD23	2:B:424:LEU:HA	1.81	0.40
2:B:296:HIS:O	2:B:300:LYS:HG3	2.21	0.40
1:C:217:ARG:HG3	1:C:243:TRP:NE1	2.35	0.40
1:A:250:LYS:NZ	4:A:2229:HOH:O	2.54	0.40
1:A:34:LYS:HD2	1:A:77:TYR:OH	2.21	0.40
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.85	0.40
1:C:72:THR:O	2:D:296:HIS:HE1	2.04	0.40
1:C:240:PHE:HD2	4:C:2119:HOH:O	2.02	0.40
1:C:72:THR:HG22	1:C:74:ASN:ND2	2.37	0.40
2:B:407:GLN:O	2:B:411:GLU:HG2	2.22	0.40
1:C:101:LEU:HB3	1:C:102:PRO:CD	2.52	0.40
2:D:262:LEU:HD11	2:D:266:LYS:HE3	2.03	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	294/303 (97%)	280 (95%)	8 (3%)	6 (2%)	7 3
1	C	294/303 (97%)	265 (90%)	18 (6%)	11 (4%)	3 1
2	B	256/258 (99%)	251 (98%)	3 (1%)	2 (1%)	19 13
2	D	256/258 (99%)	230 (90%)	22 (9%)	4 (2%)	9 4
All	All	1100/1122 (98%)	1026 (93%)	51 (5%)	23 (2%)	7 2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	293	VAL
1	A	294	PRO
1	C	38	ASP
1	C	39	THR
2	D	346	PRO
2	B	324	PRO
1	C	164	VAL
1	C	294	PRO
1	C	295	HIS
2	D	420	GLY
1	A	164	VAL
2	B	346	PRO
1	C	155	PRO
1	C	181	SER
1	C	199	ARG
1	A	40	GLU
1	C	145	ASP
1	A	295	HIS
1	C	41	THR
2	D	421	VAL
1	C	220	GLY
2	D	372	TRP

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	261/265 (98%)	236 (90%)	25 (10%)	8 5
1	C	261/265 (98%)	232 (89%)	29 (11%)	6 3
2	B	232/232 (100%)	218 (94%)	14 (6%)	19 14
2	D	232/232 (100%)	211 (91%)	21 (9%)	9 5
All	All	986/994 (99%)	897 (91%)	89 (9%)	9 6

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	12	GLU
1	A	40	GLU
1	A	45	PRO
1	A	55	LEU
1	A	72	THR
1	A	73	GLU
1	A	74	ASN
1	A	83	LEU
1	A	101	LEU
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	155	PRO
1	A	163	VAL
1	A	200	ARG
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	273	LYS
1	A	278	LYS
1	A	294	PRO
1	A	295	HIS
1	A	296	LEU
2	B	179	HIS
2	B	200	MET
2	B	202	LYS
2	B	209	SER
2	B	232	LEU

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Mol	Chain	Res	Type
2	B	292	LEU
2	B	316	THR
2	B	324	PRO
2	B	374	GLU
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	423	LEU
2	B	428	GLU
1	C	0	SER
1	C	2	GLU
1	C	9	LYS
1	C	12	GLU
1	C	17	VAL
1	C	40	GLU
1	C	41	THR
1	C	59	ASN
1	C	73	GLU
1	C	74	ASN
1	C	83	LEU
1	C	94	SER
1	C	101	LEU
1	C	122	ARG
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	199	ARG
1	C	200	ARG
1	C	206	ASP
1	C	217	ARG
1	C	226	VAL
1	C	230	VAL
1	C	232	SER
1	C	250	LYS
1	C	264	SER
1	C	278	LYS
1	C	296	LEU
2	D	177	ASP
2	D	194	LYS
2	D	197	VAL
2	D	202	LYS

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Mol	Chain	Res	Type
2	D	210	MET
2	D	245	SER
2	D	268	GLU
2	D	316	THR
2	D	324	PRO
2	D	331	SER
2	D	339	LEU
2	D	346	PRO
2	D	362	LEU
2	D	366	THR
2	D	368	THR
2	D	377	ILE
2	D	386	SER
2	D	391	LEU
2	D	397	THR
2	D	398	TYR
2	D	418	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS
1	A	131	GLN
1	A	161	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	62	ASN
1	C	85	GLN
1	C	119	HIS
1	C	131	GLN
2	D	179	HIS
2	D	254	GLN

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Mol	Chain	Res	Type
2	D	313	GLN
2	D	322	GLN
2	D	361	HIS
2	D	403	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	TPO	C	160	1	8,10,11	2.29	2 (25%)	10,14,16	1.55	3 (30%)
1	TPO	A	160	1	8,10,11	1.59	2 (25%)	10,14,16	1.43	2 (20%)

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	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	4.28	1.64	1.50
1	C	160	TPO	P-OG1	4.06	1.67	1.59
1	A	160	TPO	CG2-CB	2.68	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	2.50	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	TPO	O-C-CA	-2.90	117.18	124.78
1	C	160	TPO	P-OG1-CB	-2.83	114.67	123.21
1	C	160	TPO	O3P-P-O2P	2.19	116.03	107.64
1	C	160	TPO	O-C-CA	-2.04	119.44	124.78
1	A	160	TPO	P-OG1-CB	-2.03	117.06	123.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	6CP	A	1298[B]	-	25,28,28	1.68	6 (24%)	29,38,38	3.64	11 (37%)
3	6CP	C	1298[B]	-	25,28,28	21.15	6 (24%)	29,38,38	12.73	15 (51%)
3	6CP	C	1298[A]	-	25,28,28	1.95	5 (20%)	29,38,38	3.55	13 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6CP	A	1298[A]	-	25,28,28	1.69	6 (24%)	29,38,38	3.24	8 (27%)

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	6CP	A	1298[B]	-	-	2/9/17/17	0/4/4/4
3	6CP	C	1298[B]	-	-	0/9/17/17	0/4/4/4
3	6CP	C	1298[A]	-	-	0/9/17/17	0/4/4/4
3	6CP	A	1298[A]	-	-	0/9/17/17	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298[B]	6CP	C19-CL1	105.30	4.03	1.74
3	C	1298[B]	6CP	C4-N3	4.52	1.45	1.36
3	C	1298[A]	6CP	C4-N3	4.52	1.45	1.36
3	C	1298[B]	6CP	C2-N1	4.09	1.47	1.34
3	C	1298[A]	6CP	C2-N1	4.09	1.47	1.34
3	C	1298[B]	6CP	C6-N1	-3.88	1.24	1.31
3	C	1298[A]	6CP	C6-N1	-3.88	1.24	1.31
3	A	1298[B]	6CP	C2-N1	3.77	1.46	1.34
3	A	1298[A]	6CP	C2-N1	3.77	1.46	1.34
3	A	1298[B]	6CP	C4-N3	3.71	1.43	1.36
3	A	1298[A]	6CP	C4-N3	3.71	1.43	1.36
3	A	1298[B]	6CP	C2-N2	-3.20	1.30	1.36
3	A	1298[A]	6CP	C2-N2	-3.04	1.30	1.36
3	C	1298[B]	6CP	C5-C4	-2.80	1.33	1.40
3	C	1298[A]	6CP	C5-C4	-2.80	1.33	1.40
3	A	1298[B]	6CP	C14-C13	2.47	1.61	1.51
3	A	1298[A]	6CP	C14-C13	2.47	1.61	1.51
3	A	1298[B]	6CP	C17-N2	-2.43	1.35	1.40
3	A	1298[A]	6CP	C17-N2	-2.38	1.35	1.40
3	C	1298[B]	6CP	C2-N3	-2.26	1.28	1.34
3	C	1298[A]	6CP	C2-N3	-2.26	1.28	1.34
3	A	1298[B]	6CP	C5-C4	-2.17	1.35	1.40
3	A	1298[A]	6CP	C5-C4	-2.17	1.35	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1298[B]	6CP	C20-C19-CL1	-64.50	18.52	119.35
3	C	1298[B]	6CP	C18-C19-CL1	-13.17	102.69	119.15
3	A	1298[B]	6CP	C10-O6-C6	-12.97	105.11	117.50
3	A	1298[A]	6CP	C10-O6-C6	-12.97	105.11	117.50
3	C	1298[B]	6CP	O6-C6-N1	9.40	128.24	120.12
3	C	1298[A]	6CP	O6-C6-N1	9.40	128.24	120.12
3	C	1298[B]	6CP	N3-C2-N1	-7.72	114.02	126.23
3	C	1298[A]	6CP	N3-C2-N1	-7.72	114.02	126.23
3	C	1298[B]	6CP	C2-N1-C6	7.56	128.51	115.18
3	C	1298[A]	6CP	C2-N1-C6	7.56	128.51	115.18
3	C	1298[B]	6CP	C2-N3-C4	6.49	122.65	115.28
3	C	1298[A]	6CP	C2-N3-C4	6.49	122.65	115.28
3	A	1298[B]	6CP	C17-C18-C19	6.28	123.66	118.69
3	A	1298[B]	6CP	C2-N3-C4	6.06	122.16	115.28
3	A	1298[A]	6CP	C2-N3-C4	6.06	122.16	115.28
3	A	1298[B]	6CP	C4-C5-N7	-5.62	103.54	109.40
3	A	1298[A]	6CP	C4-C5-N7	-5.62	103.54	109.40
3	A	1298[B]	6CP	C18-C19-CL1	5.61	126.16	119.15
3	A	1298[B]	6CP	N3-C2-N1	-4.83	118.60	126.23
3	A	1298[A]	6CP	N3-C2-N1	-4.83	118.60	126.23
3	C	1298[B]	6CP	C4-C5-N7	-4.62	104.58	109.40
3	C	1298[A]	6CP	C4-C5-N7	-4.62	104.58	109.40
3	C	1298[B]	6CP	N2-C2-N3	4.25	131.36	116.92
3	C	1298[A]	6CP	N2-C2-N3	4.25	131.36	116.92
3	C	1298[B]	6CP	C5-C6-N1	-4.00	115.65	123.26
3	C	1298[A]	6CP	C5-C6-N1	-4.00	115.65	123.26
3	C	1298[B]	6CP	C14-C13-C12	3.38	118.30	111.42
3	C	1298[A]	6CP	C14-C13-C12	3.38	118.30	111.42
3	C	1298[B]	6CP	C17-N2-C2	-3.30	119.67	129.23
3	C	1298[A]	6CP	C17-N2-C2	-3.30	119.67	129.23
3	C	1298[B]	6CP	C21-C22-C17	3.26	123.62	119.72
3	C	1298[A]	6CP	C21-C22-C17	3.26	123.62	119.72
3	A	1298[B]	6CP	C20-C19-C18	-2.92	117.65	121.53
3	C	1298[B]	6CP	C17-C18-C19	2.92	121.00	118.69
3	C	1298[A]	6CP	C17-C18-C19	2.92	121.00	118.69
3	A	1298[B]	6CP	C2-N1-C6	2.89	120.27	115.18
3	A	1298[A]	6CP	C2-N1-C6	2.89	120.27	115.18
3	C	1298[B]	6CP	C22-C17-C18	-2.72	116.42	119.65
3	C	1298[A]	6CP	C22-C17-C18	-2.72	116.42	119.65
3	C	1298[B]	6CP	C13-C12-C11	-2.50	107.43	112.15
3	C	1298[A]	6CP	C13-C12-C11	-2.50	107.43	112.15
3	A	1298[B]	6CP	C14-C15-C16	2.49	116.49	111.42
3	A	1298[A]	6CP	C14-C15-C16	2.49	116.49	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1298[A]	6CP	C21-C22-C17	2.23	122.40	119.72
3	A	1298[B]	6CP	C13-C12-C11	2.23	116.37	112.15
3	A	1298[A]	6CP	C13-C12-C11	2.23	116.37	112.15
3	A	1298[B]	6CP	C20-C19-CL1	-2.04	116.17	119.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1298[B]	6CP	N3-C2-N2-C17
3	A	1298[B]	6CP	N1-C2-N2-C17

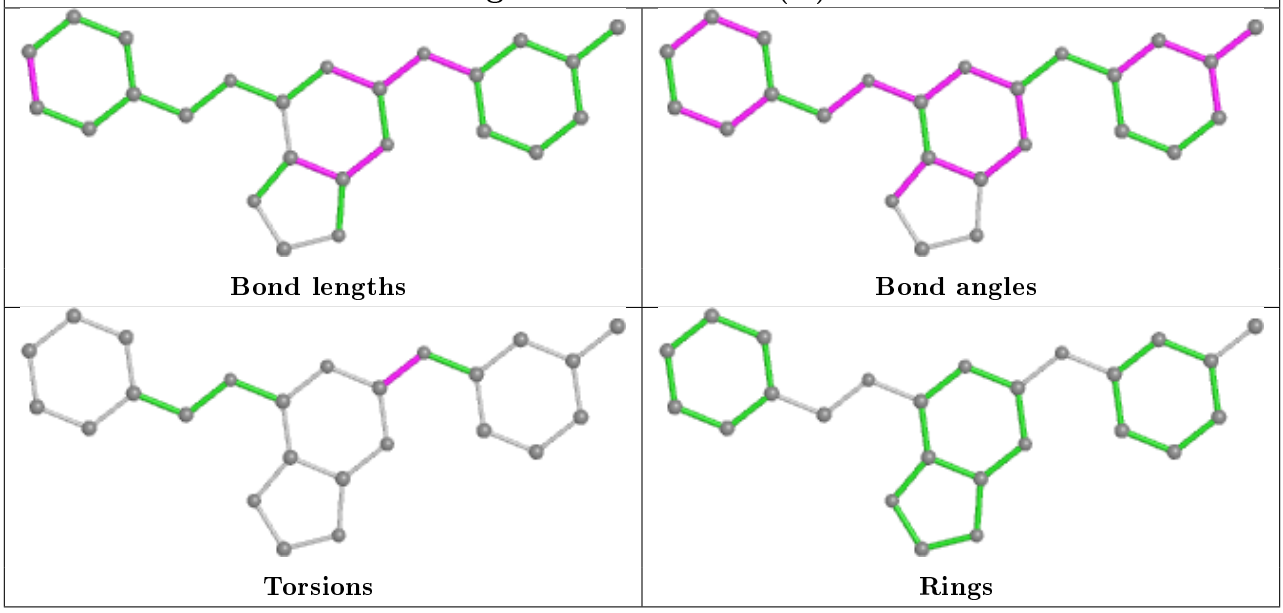
There are no ring outliers.

3 monomers are involved in 9 short contacts:

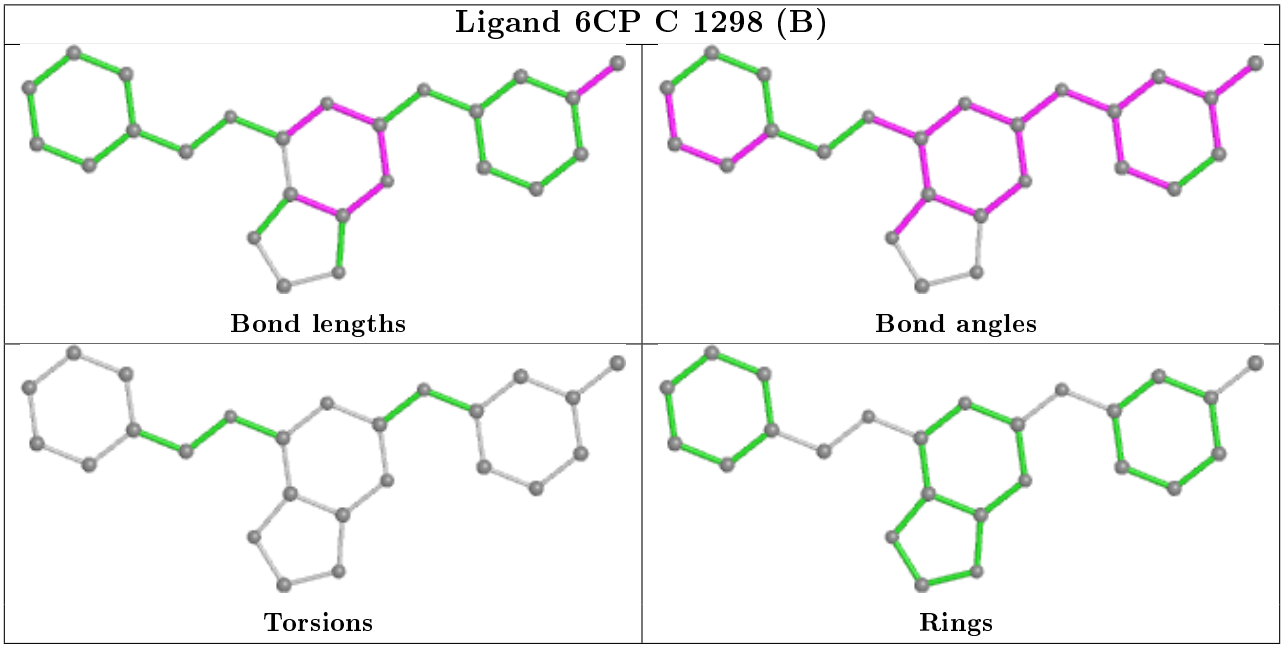
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1298[B]	6CP	4	0
3	C	1298[A]	6CP	4	0
3	A	1298[A]	6CP	1	0

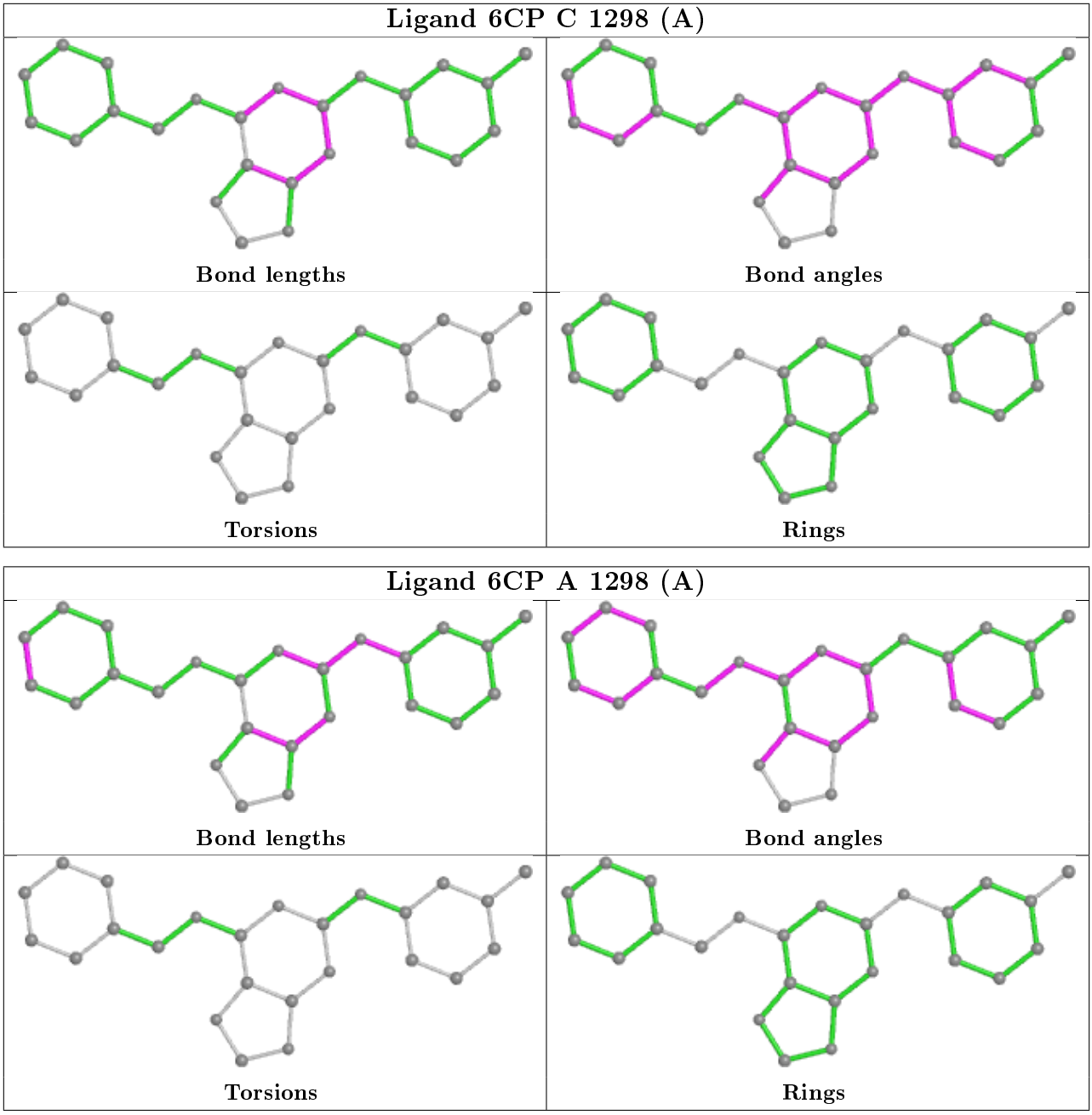
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 6CP A 1298 (B)



Ligand 6CP C 1298 (B)





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	296/303 (97%)	0.42	17 (5%) 23 23	19, 31, 61, 91	0
1	C	296/303 (97%)	1.89	94 (31%) 0 0	31, 54, 85, 99	0
2	B	258/258 (100%)	0.32	12 (4%) 31 30	21, 32, 50, 74	0
2	D	258/258 (100%)	1.55	86 (33%) 0 0	31, 58, 85, 96	0
All	All	1108/1122 (98%)	1.05	209 (18%) 1 1	19, 42, 81, 99	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	14.0
1	C	225	VAL	13.6
1	C	244	ALA	13.3
1	C	233	MET	12.2
2	B	175	VAL	11.8
1	C	296	LEU	10.9
1	C	227	TRP	10.7
1	C	236	TYR	10.7
1	C	230	VAL	10.3
1	A	295	HIS	10.3
1	C	243	TRP	9.7
1	A	40	GLU	9.0
1	C	235	ASP	8.9
1	C	232	SER	8.8
2	D	175	VAL	8.5
1	C	240	PHE	8.1
1	C	221	THR	7.6
1	C	223	ASP	7.4
1	C	231	THR	7.3
1	C	234	PRO	7.3
1	C	177	CYS	7.3

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Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	7.3
1	C	241	PRO	7.2
2	D	176	PRO	7.1
1	C	245	ARG	7.1
1	A	39	THR	7.1
2	D	367	VAL	7.0
1	C	224	GLU	6.6
2	D	423	LEU	6.6
1	C	295	HIS	6.6
1	C	249	SER	6.5
2	D	429	THR	6.4
1	C	228	PRO	6.2
2	D	430	LEU	6.1
1	C	242	LYS	6.0
1	C	247	ASP	5.7
1	C	239	SER	5.7
1	C	253	PRO	5.7
2	D	384	LEU	5.6
1	C	246	GLN	5.6
2	D	364	LEU	5.5
2	D	402	PRO	5.5
1	A	96	LEU	5.4
2	D	327	CYS	5.4
2	D	388	LYS	5.4
2	D	311	VAL	5.3
1	A	36	ARG	5.3
1	C	217	ARG	5.3
1	A	293	VAL	5.2
2	D	382	TYR	5.1
2	D	390	CYS	5.1
2	B	423	LEU	5.1
2	D	428	GLU	5.0
1	C	38	ASP	4.7
2	D	401	ALA	4.7
1	C	250	LYS	4.7
1	C	248	PHE	4.7
2	D	383	THR	4.6
1	C	238	PRO	4.6
2	D	399	LEU	4.6
1	C	294	PRO	4.6
1	C	229	GLY	4.5
1	C	256	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	419	HIS	4.4
1	C	209	ILE	4.3
2	D	431	ASN	4.3
2	B	176	PRO	4.3
2	D	425	ASN	4.2
2	D	375	SER	4.2
2	D	184	THR	4.1
1	C	175	LEU	4.1
1	C	39	THR	4.1
2	D	372	TRP	4.0
2	D	416	SER	4.0
2	D	315	LEU	3.9
2	D	177	ASP	3.9
2	D	369	GLY	3.9
2	D	324	PRO	3.9
2	D	392	MET	3.9
1	C	288	ASP	3.9
1	A	294	PRO	3.9
2	D	283	ASP	3.9
1	C	189	LEU	3.8
2	D	284	ASP	3.8
2	D	427	PRO	3.8
1	C	179	TYR	3.7
1	C	287	GLN	3.7
1	C	165	THR	3.7
1	C	161	HIS	3.6
1	A	38	ASP	3.6
2	D	379	LYS	3.6
2	D	326	ASN	3.6
1	C	271	PRO	3.6
1	C	102	PRO	3.6
1	C	101	LEU	3.6
2	D	280	TYR	3.5
2	B	283	ASP	3.5
2	D	403	GLN	3.5
2	D	391	LEU	3.5
1	C	222	PRO	3.5
2	D	328	LYS	3.4
1	C	257	GLU	3.4
1	C	128	LEU	3.4
1	C	151	ALA	3.3
1	C	218	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	3.3
2	D	365	TYR	3.3
2	D	385	GLU	3.3
1	C	41	THR	3.2
1	C	219	LEU	3.2
2	D	378	ARG	3.2
2	D	341	LEU	3.2
1	C	96	LEU	3.2
2	D	360	PHE	3.2
2	D	417	LYS	3.2
2	D	395	HIS	3.1
2	D	323	GLN	3.1
2	D	376	LEU	3.1
1	C	273	LYS	3.1
2	D	413	TYR	3.1
1	C	171	PRO	3.1
2	B	284	ASP	3.1
2	D	325	ALA	3.0
1	C	97	THR	3.0
1	A	95	ALA	3.0
2	D	415	ASN	2.9
1	C	251	VAL	2.9
2	B	323	GLN	2.9
2	D	334	MET	2.8
1	C	143	LEU	2.8
2	D	422	SER	2.8
2	D	356	ALA	2.8
2	D	320	LEU	2.8
2	D	368	THR	2.7
1	C	187	TRP	2.7
2	D	410	ARG	2.7
1	C	162	GLU	2.7
2	D	350	TYR	2.7
1	C	282	ALA	2.7
1	C	84	HIS	2.7
2	D	371	SER	2.6
2	B	431	ASN	2.6
1	C	40	GLU	2.6
1	C	199	ARG	2.6
1	A	296	LEU	2.5
2	D	358	ALA	2.5
2	B	234	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	339	LEU	2.5
2	D	387	LEU	2.5
1	C	7	VAL	2.5
1	C	99	ILE	2.5
1	C	36	ARG	2.5
2	D	336	LEU	2.5
1	C	292	PRO	2.5
2	B	236	VAL	2.5
1	C	237	LYS	2.5
1	C	260	ARG	2.4
1	C	269	TYR	2.4
1	C	284	PRO	2.4
2	D	363	ALA	2.4
1	C	111	LEU	2.4
2	B	324	PRO	2.4
2	D	396	GLN	2.4
1	C	133	LEU	2.3
1	A	19	TYR	2.3
1	C	123	VAL	2.3
1	C	220	GLY	2.3
1	C	15	TYR	2.3
1	A	108	LEU	2.3
2	D	337	GLY	2.3
1	C	158	THR	2.3
1	C	89	LYS	2.3
1	C	286	PHE	2.2
2	D	424	LEU	2.2
2	D	180	GLU	2.2
2	D	233	HIS	2.2
2	D	202	LYS	2.2
2	D	188	GLU	2.2
2	D	404	HIS	2.2
2	D	232	LEU	2.2
2	D	178	TYR	2.2
1	C	137	THR	2.2
1	A	0	SER	2.2
1	C	168	TYR	2.2
1	C	115	LEU	2.1
2	D	225	TYR	2.1
1	C	192	ILE	2.1
1	C	283	HIS	2.1
2	D	400	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	163	VAL	2.1
2	D	235	ALA	2.1
2	D	366	THR	2.1
2	D	397	THR	2.1
1	C	255	LEU	2.1
2	D	319	PHE	2.1
1	C	124	LEU	2.1
2	D	362	LEU	2.1
1	C	94	SER	2.1
1	A	74	ASN	2.0
1	C	173	ILE	2.0
1	A	73	GLU	2.0
2	D	374	GLU	2.0
2	B	355	ILE	2.0
1	C	254	PRO	2.0
2	D	426	PRO	2.0
1	A	37	LEU	2.0
2	D	316	THR	2.0
2	B	177	ASP	2.0
2	D	197	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	C	160	11/12	0.92	0.15	34,44,50,52	0
1	TPO	A	160	11/12	0.99	0.10	24,26,27,27	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

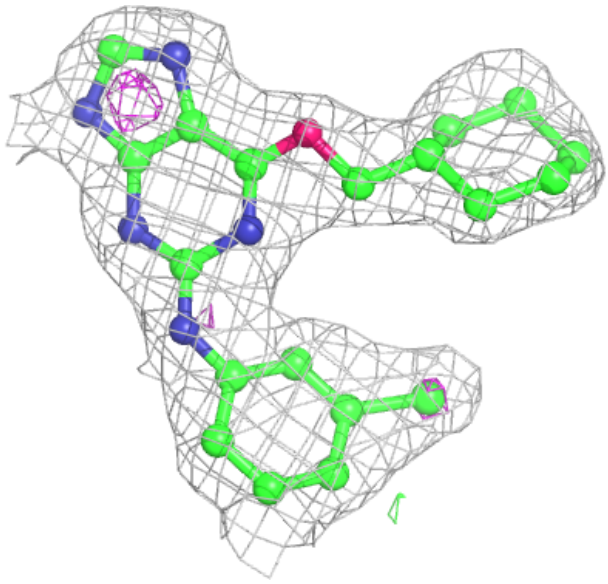
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

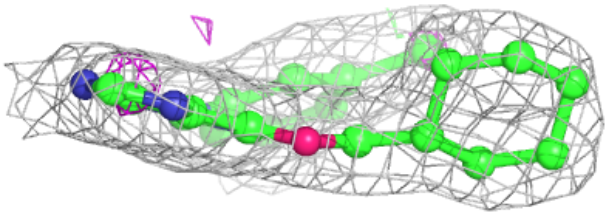
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6CP	A	1298[B]	25/25	0.92	0.15	29,34,37,37	25
3	6CP	A	1298[A]	25/25	0.92	0.15	29,35,39,40	25
3	6CP	C	1298[A]	25/25	0.93	0.16	36,42,47,48	25
3	6CP	C	1298[B]	25/25	0.93	0.16	36,42,47,48	25

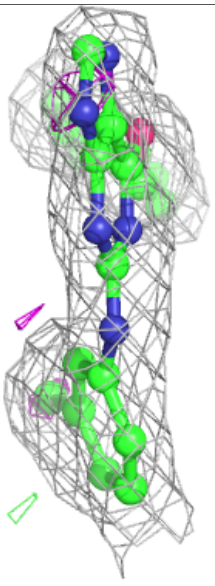
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 6CP A 1298 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

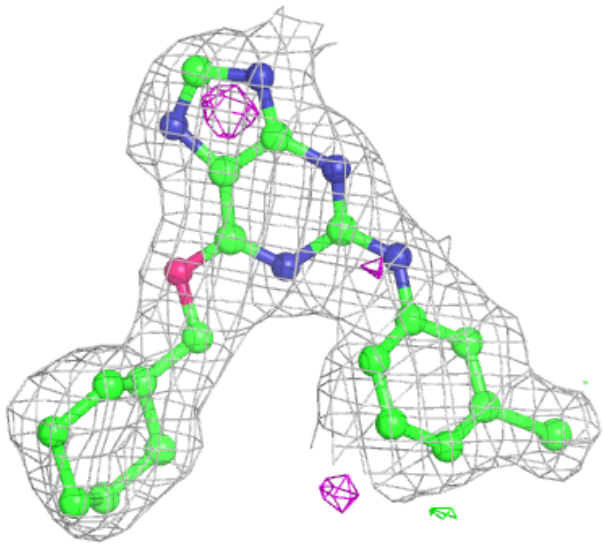


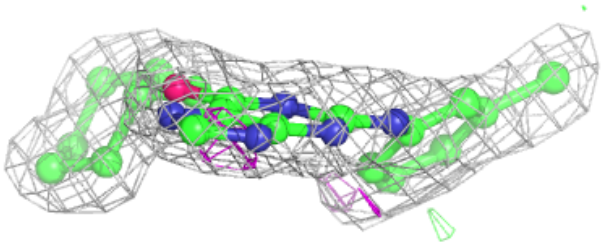


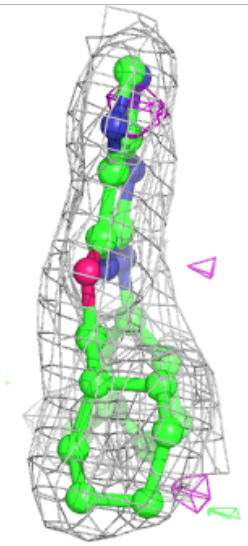


Electron density around 6CP A 1298 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

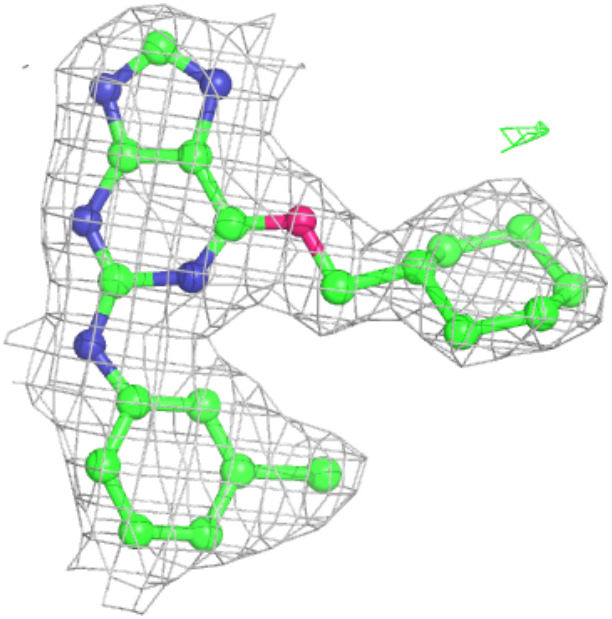


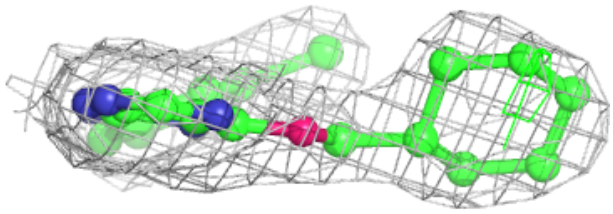


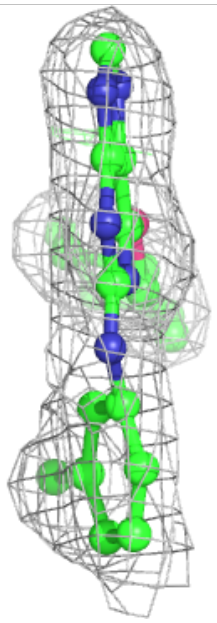


Electron density around 6CP C 1298 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

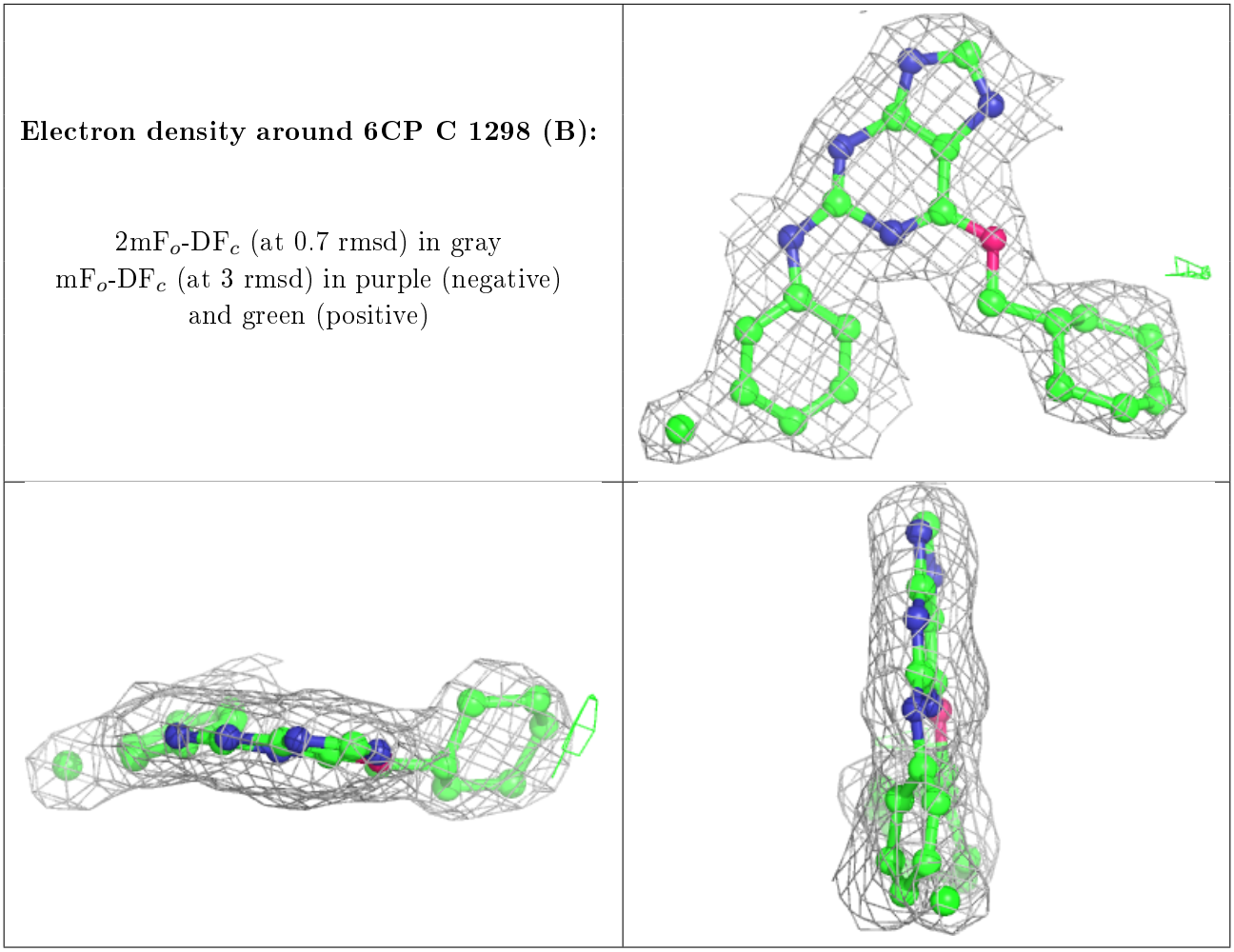






Electron density around 6CP C 1298 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.