



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:34 AM UTC

PDB ID : 1H1R / pdb_00001h1r
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

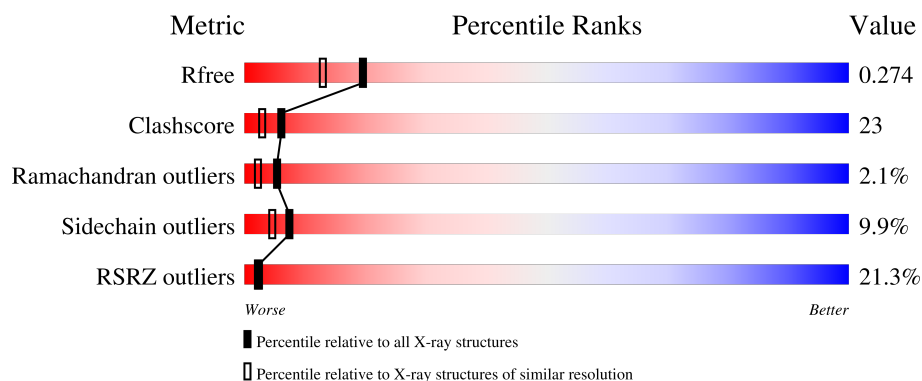
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	C	303	
2	B	258	
2	D	258	

2 Entry composition [i](#)

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.

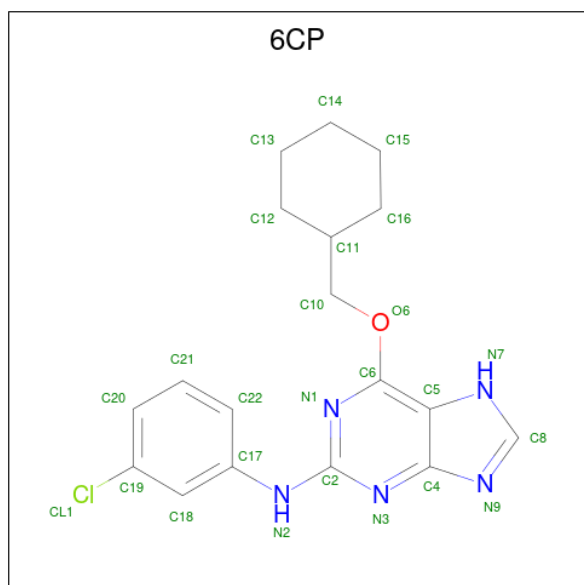
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

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 (CCD ID: 6CP) (formula: C₁₈H₂₀ClN₅O).



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

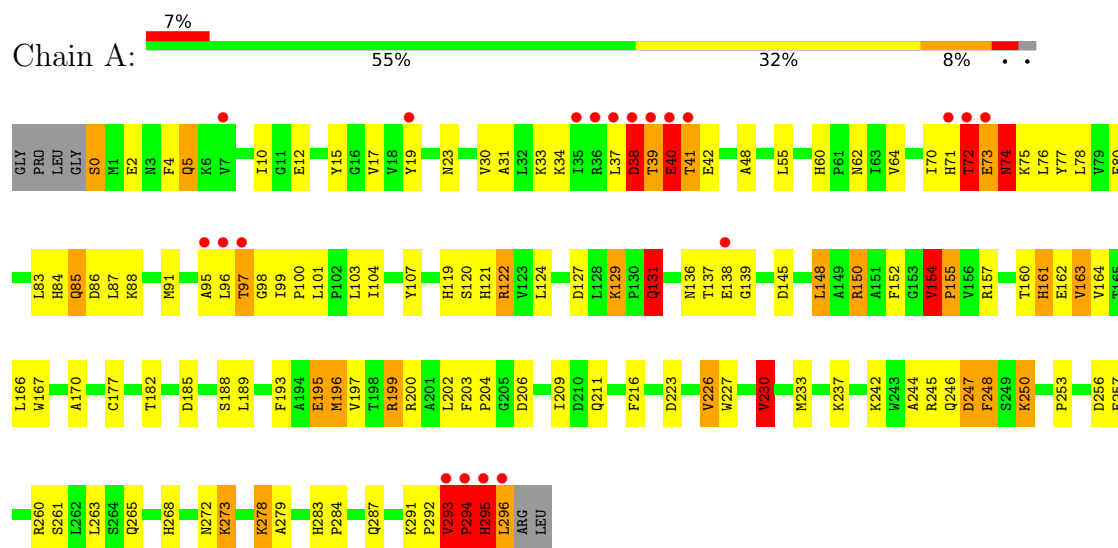
- Molecule 4 is water.

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

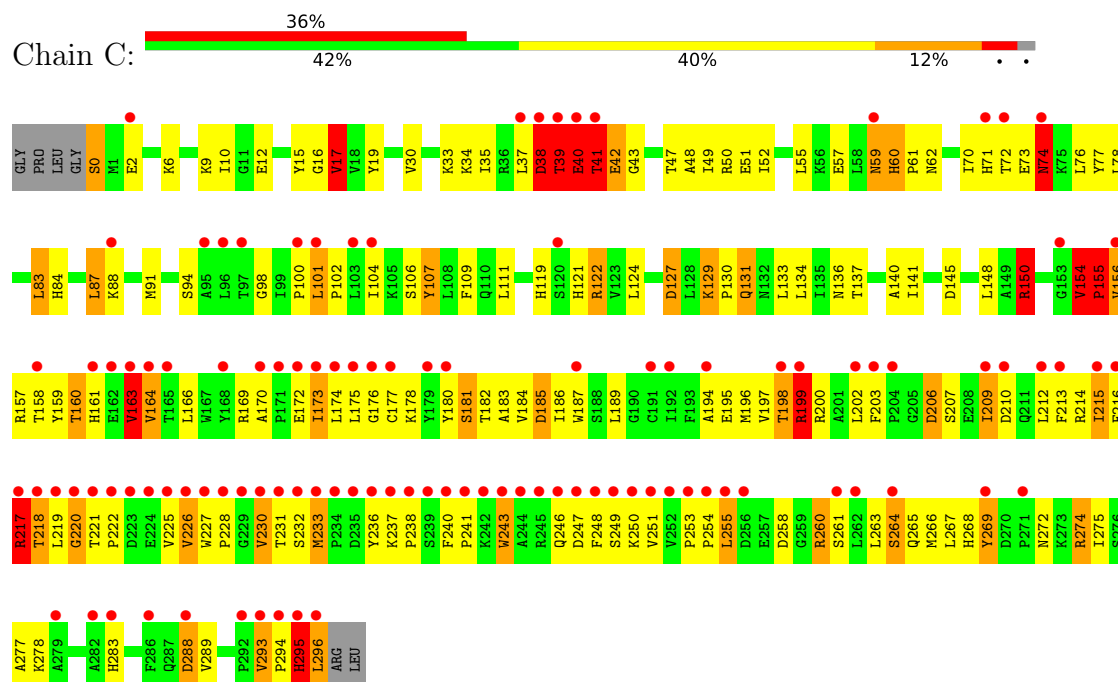
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

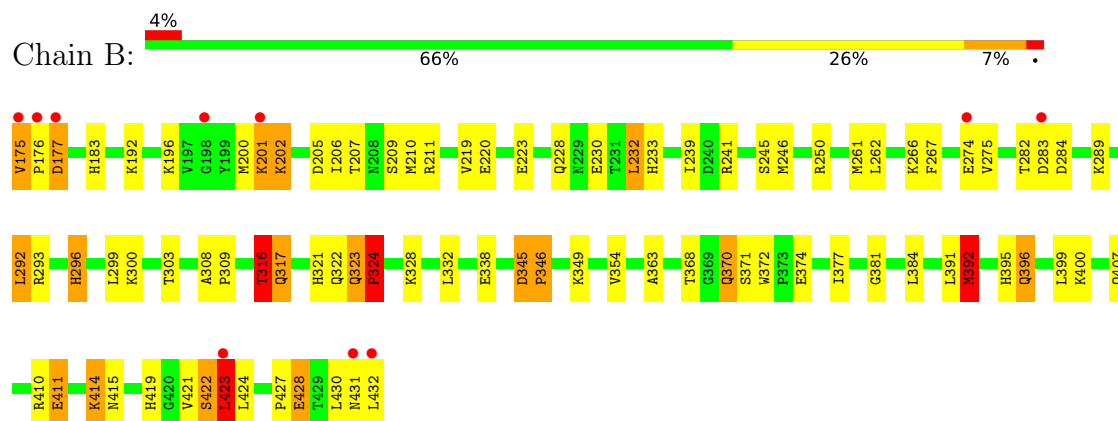
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



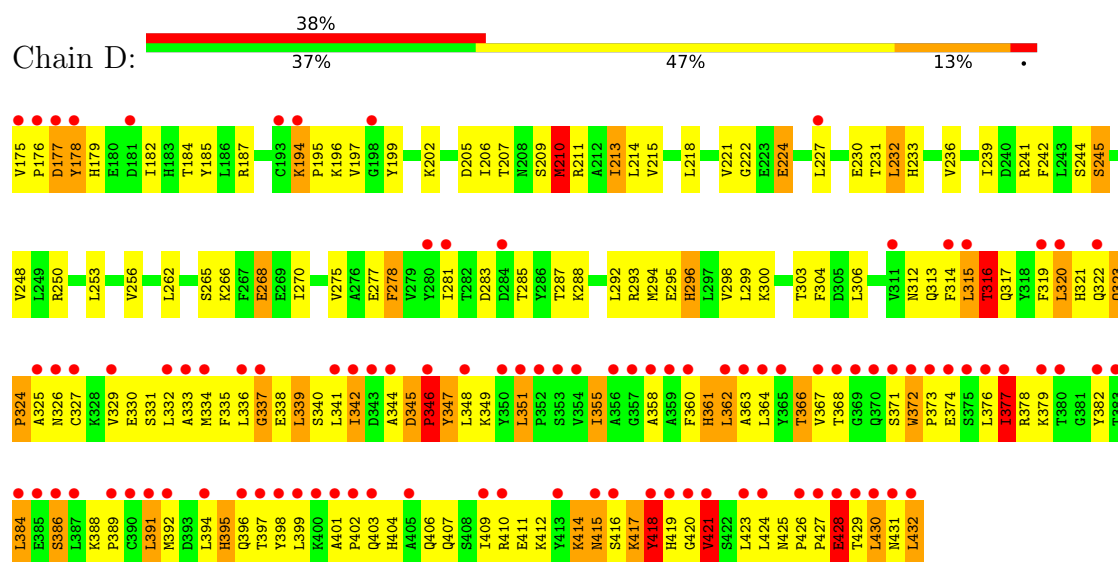
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



● Molecule 2: CYCLIN A2



● Molecule 2: CYCLIN A2



4 Data and refinement statistics

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.00) 92.6 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.40 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.15	2/2438 (0.1%)	2.54	124/3308 (3.7%)
1	C	0.80	0/2438	2.08	83/3308 (2.5%)
2	B	1.02	1/2133 (0.0%)	2.17	79/2897 (2.7%)
2	D	0.83	0/2133	2.10	71/2897 (2.5%)
All	All	0.97	3/9142 (0.0%)	2.24	357/12410 (2.9%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	VAL	N-CA	8.60	1.57	1.46
2	B	354	VAL	C-O	6.01	1.31	1.24
1	A	295	HIS	N-CA	-6.01	1.38	1.46

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	PRO	CA-C-N	29.07	177.06	121.54
1	A	294	PRO	C-N-CA	29.07	177.06	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	CD-NE-CZ	26.46	161.44	124.40
1	A	199	ARG	CD-NE-CZ	24.00	158.00	124.40
1	A	295	HIS	CA-CB-CG	23.74	137.54	113.80
1	C	217	ARG	CD-NE-CZ	23.43	157.20	124.40
1	A	250	LYS	CG-CD-CE	20.97	159.54	111.30
2	D	296	HIS	CA-CB-CG	19.69	133.49	113.80
1	A	295	HIS	N-CA-CB	19.31	143.12	110.49
2	D	323	GLN	CA-C-O	-18.44	102.28	119.62
1	A	154	VAL	CA-C-O	-18.40	106.87	119.38
1	A	295	HIS	CA-C-N	18.29	154.62	121.70
1	A	295	HIS	C-N-CA	18.29	154.62	121.70
2	D	345	ASP	CA-C-O	-17.14	96.68	120.16
2	B	323	GLN	CA-C-O	-16.84	103.39	119.55
2	B	423	LEU	CB-CA-C	16.79	139.78	111.23
2	B	345	ASP	CA-C-O	-16.66	105.49	119.99
1	A	293	VAL	N-CA-CB	-15.73	89.18	111.21
1	A	294	PRO	O-C-N	-14.45	103.13	122.64
1	C	154	VAL	CA-C-O	-14.05	101.12	119.95
1	A	230	VAL	N-CA-CB	13.99	126.04	110.51
1	A	295	HIS	CA-C-O	13.34	139.58	120.51
1	A	293	VAL	CB-CA-C	12.74	134.54	111.36
2	B	422	SER	CA-C-N	-12.70	104.25	123.17
2	B	422	SER	C-N-CA	-12.70	104.25	123.17
1	A	230	VAL	CB-CA-C	-11.76	96.82	111.88
2	D	395	HIS	CA-CB-CG	11.54	125.34	113.80
2	D	378	ARG	CD-NE-CZ	11.34	140.28	124.40
1	C	39	THR	CA-C-N	11.17	142.87	121.54
1	C	39	THR	C-N-CA	11.17	142.87	121.54
2	D	323	GLN	CA-C-N	10.98	131.67	119.92
2	D	323	GLN	C-N-CA	10.98	131.67	119.92
1	A	40	GLU	CA-C-N	10.58	138.06	120.81
1	A	40	GLU	C-N-CA	10.58	138.06	120.81
1	A	86	ASP	CA-CB-CG	10.23	122.83	112.60
1	A	295	HIS	CB-CA-C	-10.13	90.26	110.42
1	A	293	VAL	O-C-N	-10.07	109.61	121.10
2	D	253	LEU	CA-C-O	10.05	131.08	120.42
2	D	324	PRO	CA-N-CD	-9.90	98.14	112.00
1	C	40	GLU	CA-C-O	9.83	134.56	120.51
2	B	324	PRO	CA-N-CD	-9.69	98.44	112.00
2	B	205	ASP	N-CA-C	9.18	124.48	113.28
1	C	217	ARG	CB-CG-CD	9.17	132.40	111.30
2	B	323	GLN	CA-C-N	9.13	131.25	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	323	GLN	C-N-CA	9.13	131.25	119.84
1	A	163	VAL	N-CA-CB	-9.12	94.86	111.92
1	A	248	PHE	CA-CB-CG	-9.10	104.70	113.80
2	B	316	THR	N-CA-CB	-8.95	96.96	110.12
1	A	209	ILE	O-C-N	-8.78	112.78	121.83
2	B	415	ASN	CA-CB-CG	8.76	121.36	112.60
2	D	256	VAL	CA-C-O	8.69	130.38	121.17
1	A	199	ARG	NE-CZ-NH2	-8.59	111.47	119.20
1	C	154	VAL	CA-C-N	8.52	130.49	119.84
1	C	154	VAL	C-N-CA	8.52	130.49	119.84
1	C	274	ARG	CD-NE-CZ	8.51	136.31	124.40
1	A	40	GLU	CA-C-O	8.50	132.66	120.51
2	B	321	HIS	CA-CB-CG	-8.50	105.30	113.80
1	A	292	PRO	O-C-N	-8.49	112.33	122.86
2	B	411	GLU	CB-CA-C	-8.40	97.62	110.90
2	D	415	ASN	CA-CB-CG	8.40	121.00	112.60
1	C	155	PRO	CA-N-CD	-8.38	100.27	112.00
1	A	98	GLY	CA-C-N	-8.13	116.74	122.59
1	A	98	GLY	C-N-CA	-8.13	116.74	122.59
2	D	430	LEU	N-CA-C	-8.10	103.86	114.31
1	A	293	VAL	CA-CB-CG1	8.09	124.16	110.40
1	A	80	PHE	CA-CB-CG	8.09	121.89	113.80
1	C	122	ARG	CA-CB-CG	8.08	130.26	114.10
2	D	378	ARG	NE-CZ-NH2	8.05	126.44	119.20
2	B	261	MET	CA-C-N	8.04	131.06	120.28
2	B	261	MET	C-N-CA	8.04	131.06	120.28
2	D	268	GLU	N-CA-C	7.98	123.14	113.41
2	D	177	ASP	CA-CB-CG	7.96	120.56	112.60
1	A	4	PHE	CA-CB-CG	-7.92	105.88	113.80
1	C	41	THR	N-CA-C	-7.92	93.93	110.80
2	B	370	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	A	122	ARG	CA-CB-CG	7.74	129.58	114.10
1	A	41	THR	N-CA-CB	7.73	117.40	109.51
1	A	85	GLN	N-CA-CB	-7.65	99.67	111.46
1	C	295	HIS	N-CA-CB	7.65	123.42	110.49
1	C	155	PRO	N-CA-CB	7.65	111.28	103.25
2	B	419	HIS	CA-CB-CG	-7.61	106.19	113.80
1	A	272	ASN	CA-CB-CG	-7.59	105.01	112.60
2	D	355	ILE	N-CA-CB	7.58	118.92	110.51
2	D	351	LEU	CA-C-O	7.54	129.38	120.41
1	A	157	ARG	CA-CB-CG	7.52	129.15	114.10
1	C	74	ASN	CA-CB-CG	7.52	120.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	VAL	O-C-N	7.51	129.66	121.10
2	B	282	THR	CA-C-N	7.47	132.97	122.36
2	B	282	THR	C-N-CA	7.47	132.97	122.36
1	A	155	PRO	CA-N-CD	-7.41	101.63	112.00
1	C	260	ARG	CD-NE-CZ	7.40	134.76	124.40
1	A	161	HIS	CB-CG-ND1	7.38	133.78	122.70
1	A	188	SER	CA-C-O	7.36	128.55	120.82
1	A	120	SER	CA-CB-OG	-7.30	96.49	111.10
1	A	96	LEU	N-CA-C	-7.28	104.01	113.12
1	C	50	ARG	CD-NE-CZ	-7.25	114.25	124.40
2	D	324	PRO	N-CA-C	7.21	122.51	111.34
1	C	39	THR	N-CA-CB	7.19	122.64	110.49
1	A	161	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	74	ASN	CA-CB-CG	7.13	119.73	112.60
1	A	162	GLU	O-C-N	7.10	130.91	122.46
1	C	17	VAL	CB-CA-C	-7.06	99.95	110.82
1	C	47	THR	CA-CB-OG1	-7.06	99.01	109.60
2	D	293	ARG	CD-NE-CZ	7.05	134.27	124.40
2	B	377	ILE	CA-C-O	7.04	128.31	120.85
2	D	346	PRO	CA-N-CD	-7.02	102.17	112.00
2	D	221	VAL	CB-CA-C	-7.00	103.01	111.97
2	B	396	GLN	OE1-CD-NE2	-6.97	115.63	122.60
1	A	293	VAL	CA-C-N	6.91	128.48	119.84
1	A	293	VAL	C-N-CA	6.91	128.48	119.84
2	D	384	LEU	N-CA-C	-6.90	102.99	113.89
1	A	30	VAL	CA-C-O	-6.89	114.89	121.64
2	B	377	ILE	O-C-N	-6.89	114.73	121.83
1	A	72	THR	N-CA-CB	-6.84	100.50	110.70
2	B	354	VAL	CA-C-N	6.84	129.17	120.56
2	B	354	VAL	C-N-CA	6.84	129.17	120.56
1	A	166	LEU	CA-C-O	-6.82	113.27	120.63
2	B	175	VAL	CA-C-N	6.82	127.78	120.83
2	B	175	VAL	C-N-CA	6.82	127.78	120.83
1	C	74	ASN	OD1-CG-ND2	-6.82	115.78	122.60
2	B	345	ASP	O-C-N	6.80	128.04	120.83
1	A	193	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	87	LEU	CA-C-O	-6.77	113.37	120.55
1	A	157	ARG	CD-NE-CZ	6.76	133.87	124.40
2	D	373	PRO	N-CA-C	6.76	121.44	111.03
2	B	399	LEU	O-C-N	6.76	129.28	122.12
2	B	228	GLN	OE1-CD-NE2	-6.75	115.85	122.60
2	D	347	TYR	N-CA-C	6.74	121.33	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	158	THR	N-CA-C	-6.69	100.38	110.28
1	A	41	THR	N-CA-C	-6.67	100.82	108.49
2	B	346	PRO	N-CA-CB	6.65	109.91	102.60
1	A	152	PHE	CA-CB-CG	6.63	120.43	113.80
2	B	176	PRO	N-CA-C	6.62	121.56	114.68
2	D	265	SER	CA-C-O	6.56	127.37	120.42
2	D	414	LYS	N-CA-C	-6.54	105.88	114.31
2	B	196	LYS	CA-C-N	6.50	128.99	120.60
2	B	196	LYS	C-N-CA	6.50	128.99	120.60
1	C	215	ILE	CB-CA-C	6.46	119.88	111.81
2	D	406	GLN	CB-CG-CD	6.46	123.58	112.60
1	C	206	ASP	CA-CB-CG	-6.44	106.16	112.60
1	C	121	HIS	CA-CB-CG	-6.43	107.37	113.80
2	B	201	LYS	CA-CB-CG	6.40	126.89	114.10
1	A	245	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	C	269	TYR	CB-CA-C	-6.35	100.91	110.88
1	A	154	VAL	CB-CA-C	6.34	117.16	110.37
2	D	285	THR	CA-C-O	6.34	127.27	119.79
1	C	40	GLU	N-CA-CB	6.33	121.19	110.49
1	A	129	LYS	N-CA-C	-6.29	102.56	108.22
1	C	226	VAL	CA-C-N	-6.28	114.21	122.74
1	C	226	VAL	C-N-CA	-6.28	114.21	122.74
1	A	38	ASP	CA-C-N	6.27	133.52	121.54
1	A	38	ASP	C-N-CA	6.27	133.52	121.54
1	A	145	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	202	LEU	CA-C-O	6.24	127.16	120.55
1	A	154	VAL	CA-C-N	6.23	127.63	119.84
1	A	154	VAL	C-N-CA	6.23	127.63	119.84
2	B	192	LYS	CA-C-O	-6.20	112.84	119.97
1	C	268	HIS	CA-CB-CG	6.19	119.99	113.80
2	B	381	GLY	N-CA-C	-6.18	107.18	115.21
1	C	207	SER	CA-C-O	-6.18	114.67	121.28
1	A	253	PRO	N-CA-C	6.13	118.19	110.70
2	B	316	THR	CB-CA-C	6.12	120.96	110.79
1	A	250	LYS	CB-CG-CD	6.11	125.35	111.30
2	B	349	LYS	CA-CB-CG	6.11	126.31	114.10
2	B	296	HIS	CA-CB-CG	6.09	119.89	113.80
2	B	346	PRO	CA-N-CD	-6.09	102.97	111.50
2	D	241	ARG	NH1-CZ-NH2	6.09	127.21	119.30
2	B	432	LEU	CA-C-O	-6.08	110.47	120.80
1	A	73	GLU	CA-CB-CG	6.06	126.22	114.10
2	D	361	HIS	CA-CB-CG	6.06	119.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLN	OE1-CD-NE2	-6.05	116.55	122.60
2	B	370	GLN	CA-CB-CG	6.05	126.19	114.10
2	B	223	GLU	CB-CG-CD	-6.04	102.33	112.60
1	A	99	ILE	CA-C-O	6.03	122.71	119.15
2	D	296	HIS	N-CA-CB	-6.02	101.03	110.30
2	D	417	LYS	CA-C-O	-6.02	114.13	120.63
2	D	331	SER	CA-C-O	-6.01	114.14	120.63
1	C	203	PHE	N-CA-C	5.98	119.46	108.94
1	A	74	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	157	ARG	CB-CA-C	-5.95	99.69	111.60
1	A	121	HIS	CA-CB-CG	-5.94	107.86	113.80
1	C	16	GLY	N-CA-C	5.94	123.09	112.22
2	D	210	MET	O-C-N	-5.93	115.83	122.12
2	D	355	ILE	N-CA-C	-5.91	104.16	110.36
1	A	279	ALA	CA-C-O	5.89	126.67	120.42
1	C	156	VAL	CA-C-O	-5.88	116.21	121.97
1	A	166	LEU	N-CA-C	5.88	118.44	111.33
1	A	263	LEU	O-C-N	-5.86	115.90	122.12
2	B	423	LEU	O-C-N	-5.86	114.06	121.97
2	D	294	MET	O-C-N	-5.85	115.92	122.12
1	A	31	ALA	O-C-N	-5.84	116.67	123.27
1	C	293	VAL	N-CA-CB	-5.84	103.03	111.21
2	B	296	HIS	N-CA-CB	-5.84	101.53	110.12
2	B	245	SER	CA-CB-OG	-5.84	99.43	111.10
2	D	241	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	C	198	THR	O-C-N	-5.82	116.07	122.07
2	B	177	ASP	CA-CB-CG	5.82	118.42	112.60
2	B	205	ASP	CA-CB-CG	-5.82	106.78	112.60
1	C	129	LYS	N-CA-CB	5.81	118.73	111.35
1	C	198	THR	CA-C-O	5.81	126.92	120.82
2	D	377	ILE	CA-C-O	5.79	126.72	120.47
2	D	277	GLU	CB-CG-CD	5.79	122.44	112.60
1	C	163	VAL	O-C-N	-5.78	116.81	123.00
2	D	287	THR	N-CA-C	-5.78	103.08	110.53
1	C	124	LEU	CA-C-N	5.77	130.23	120.88
1	C	124	LEU	C-N-CA	5.77	130.23	120.88
1	A	295	HIS	O-C-N	-5.76	114.92	122.59
2	B	220	GLU	CB-CA-C	-5.75	101.85	110.88
1	C	209	ILE	N-CA-CB	5.74	116.64	110.62
1	C	283	HIS	CA-C-N	5.74	126.12	119.47
1	C	283	HIS	C-N-CA	5.74	126.12	119.47
1	A	39	THR	N-CA-CB	5.73	120.18	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	ASN	OD1-CG-ND2	5.72	128.32	122.60
1	C	156	VAL	CB-CA-C	-5.72	103.87	111.13
1	C	166	LEU	CA-C-N	5.72	129.84	120.63
1	C	166	LEU	C-N-CA	5.72	129.84	120.63
2	B	241	ARG	CA-C-O	-5.68	113.09	119.79
2	B	324	PRO	N-CA-CB	5.68	109.21	103.25
1	C	173	ILE	CA-C-N	5.66	128.14	120.38
1	C	173	ILE	C-N-CA	5.66	128.14	120.38
1	C	175	LEU	CA-C-O	5.66	125.97	119.35
2	B	196	LYS	CB-CA-C	5.65	119.56	110.29
2	D	185	TYR	CA-C-O	5.64	126.93	120.90
1	A	127	ASP	CA-CB-CG	-5.64	106.96	112.60
2	B	220	GLU	N-CA-CB	5.63	118.18	110.01
1	A	203	PHE	CA-CB-CG	5.63	119.43	113.80
2	B	346	PRO	N-CD-CG	5.62	110.54	103.80
1	C	247	ASP	CA-CB-CG	-5.61	106.99	112.60
2	D	245	SER	CB-CA-C	-5.61	99.94	109.03
1	A	278	LYS	N-CA-CB	-5.60	101.89	110.01
1	A	84	HIS	N-CA-C	5.60	119.29	112.23
1	A	97	THR	N-CA-C	5.60	120.23	112.45
1	A	246	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	C	87	LEU	CA-C-N	5.59	127.71	120.44
1	C	87	LEU	C-N-CA	5.59	127.71	120.44
2	D	294	MET	CA-C-O	5.59	126.48	120.55
2	D	315	LEU	O-C-N	-5.59	115.68	122.11
2	B	324	PRO	N-CD-CG	5.59	111.58	103.20
1	C	185	ASP	CA-CB-CG	5.58	118.18	112.60
2	B	202	LYS	N-CA-C	-5.57	106.38	114.12
1	C	127	ASP	CA-C-N	-5.57	113.23	121.24
1	C	127	ASP	C-N-CA	-5.57	113.23	121.24
2	D	377	ILE	N-CA-C	-5.56	104.14	111.09
2	D	342	ILE	CB-CA-C	-5.56	104.64	112.14
2	D	213	ILE	CB-CA-C	-5.55	104.78	111.88
2	D	224	GLU	CA-CB-CG	5.55	125.19	114.10
2	D	295	GLU	N-CA-CB	5.55	118.20	109.94
1	C	173	ILE	N-CA-C	-5.54	105.45	110.82
2	B	338	GLU	CB-CG-CD	5.54	122.01	112.60
1	A	104	ILE	O-C-N	5.53	127.33	121.91
1	C	172	GLU	CB-CG-CD	5.53	122.00	112.60
2	D	210	MET	CB-CA-C	5.52	119.96	110.79
2	D	242	PHE	O-C-N	-5.52	116.39	122.07
1	A	189	LEU	CA-C-N	5.51	126.06	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	LEU	C-N-CA	5.51	126.06	120.00
2	D	221	VAL	N-CA-CB	5.51	116.99	110.55
1	A	195	GLU	O-C-N	-5.50	115.78	122.22
1	A	257	GLU	N-CA-C	5.49	117.97	111.33
2	B	399	LEU	CA-C-O	-5.48	114.74	120.55
2	D	337	GLY	N-CA-C	-5.48	106.16	112.73
2	D	253	LEU	O-C-N	-5.47	115.91	122.15
2	B	239	ILE	CA-C-O	-5.46	114.98	121.05
1	C	226	VAL	N-CA-CB	5.46	117.19	110.64
2	B	220	GLU	CA-C-O	-5.46	115.09	120.82
2	B	423	LEU	CB-CG-CD1	5.45	127.05	110.70
1	A	104	ILE	CA-C-O	-5.45	115.39	121.17
1	A	23	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	288	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	247	ASP	N-CA-CB	-5.43	100.93	109.51
1	A	244	ALA	O-C-N	-5.42	116.27	122.89
2	D	199	TYR	CA-CB-CG	5.42	123.66	113.90
1	A	197	VAL	CB-CA-C	-5.41	104.95	112.04
2	D	421	VAL	CA-C-O	-5.41	114.02	120.78
1	A	30	VAL	CA-CB-CG2	5.41	119.60	110.40
2	D	178	TYR	CA-CB-CG	-5.41	104.17	113.90
1	A	248	PHE	CA-C-O	-5.40	114.15	120.20
1	C	163	VAL	CB-CA-C	5.40	119.33	110.69
2	D	283	ASP	N-CA-CB	5.38	119.67	111.70
1	A	256	ASP	CA-C-O	-5.38	115.76	121.94
2	D	268	GLU	N-CA-CB	-5.37	102.63	110.47
2	D	205	ASP	CA-CB-CG	5.37	117.97	112.60
2	D	253	LEU	N-CA-C	5.36	117.20	111.36
2	B	317	GLN	CB-CG-CD	-5.35	103.50	112.60
1	C	157	ARG	CD-NE-CZ	5.35	131.89	124.40
1	A	263	LEU	CA-C-O	5.34	126.21	120.55
1	A	124	LEU	CA-C-O	-5.34	114.61	120.43
1	A	211	GLN	CA-C-N	5.34	127.38	120.44
1	A	211	GLN	C-N-CA	5.34	127.38	120.44
2	B	303	THR	N-CA-CB	5.34	119.60	111.70
2	B	377	ILE	N-CA-C	-5.34	105.33	110.72
1	C	150	ARG	CA-CB-CG	5.33	124.77	114.10
2	D	278	PHE	CA-C-O	-5.33	114.89	120.55
1	A	293	VAL	CA-C-O	-5.30	112.84	119.95
2	B	414	LYS	N-CA-C	-5.30	106.32	112.89
1	C	107	TYR	CA-C-O	-5.30	114.98	120.92
1	A	170	ALA	CA-C-N	5.30	124.93	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ALA	C-N-CA	5.30	124.93	119.05
1	A	150	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	A	216	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	73	GLU	CA-C-N	5.29	133.22	121.80
1	A	73	GLU	C-N-CA	5.29	133.22	121.80
2	B	267	PHE	O-C-N	-5.29	116.63	122.07
1	A	19	TYR	CB-CA-C	-5.28	99.41	109.66
1	C	155	PRO	N-CD-CG	5.27	111.10	103.20
2	B	176	PRO	CB-CA-C	-5.26	103.36	110.52
2	D	298	VAL	N-CA-CB	5.26	116.71	110.55
1	A	100	PRO	CA-C-O	5.26	127.30	121.36
1	A	2	GLU	N-CA-C	5.26	117.01	111.28
1	C	206	ASP	OD1-CG-OD2	5.24	135.48	122.90
1	C	60	HIS	CA-C-N	5.24	124.90	119.56
1	C	60	HIS	C-N-CA	5.24	124.90	119.56
2	B	316	THR	OG1-CB-CG2	5.23	119.77	109.30
1	C	199	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	D	316	THR	N-CA-CB	-5.23	101.88	110.14
1	A	279	ALA	O-C-N	-5.22	116.19	122.15
1	C	233	MET	CA-C-N	5.22	124.84	119.05
1	C	233	MET	C-N-CA	5.22	124.84	119.05
2	B	274	GLU	CA-C-O	-5.22	115.66	121.81
2	B	322	GLN	CA-C-O	-5.21	115.32	121.16
2	D	432	LEU	CA-C-O	-5.20	111.96	120.80
2	D	418	TYR	CA-CB-CG	5.19	123.24	113.90
1	C	42	GLU	N-CA-CB	-5.19	102.32	110.46
1	C	258	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	382	TYR	CA-C-O	-5.19	114.78	120.43
2	B	299	LEU	CA-C-O	5.18	126.26	120.82
1	A	87	LEU	O-C-N	5.18	127.61	122.12
2	B	411	GLU	N-CA-CB	5.18	117.58	110.07
2	D	323	GLN	CB-CA-C	5.16	117.36	110.13
1	C	70	ILE	CB-CA-C	5.16	118.24	111.53
1	A	196	MET	CA-C-N	5.15	128.10	120.74
1	A	196	MET	C-N-CA	5.15	128.10	120.74
1	A	64	VAL	N-CA-CB	5.13	116.83	110.05
1	A	157	ARG	N-CA-C	-5.12	102.43	110.17
2	B	421	VAL	O-C-N	-5.11	116.24	122.06
2	D	428	GLU	N-CA-C	-5.11	106.21	112.90
2	B	354	VAL	O-C-N	-5.09	116.58	121.83
1	A	72	THR	CB-CA-C	5.09	119.42	110.36
1	A	38	ASP	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	239	ILE	CA-C-O	-5.08	115.78	121.17
2	B	230	GLU	CA-C-N	5.08	127.04	120.44
2	B	230	GLU	C-N-CA	5.08	127.04	120.44
2	B	246	MET	CA-C-N	5.08	128.06	120.95
2	B	246	MET	C-N-CA	5.08	128.06	120.95
1	C	30	VAL	N-CA-CB	-5.08	106.05	112.60
2	D	248	VAL	CA-C-O	-5.07	114.98	120.36
1	A	122	ARG	CD-NE-CZ	5.07	131.49	124.40
2	B	392	MET	CG-SD-CE	5.07	112.04	100.90
1	C	163	VAL	N-CA-CB	-5.07	102.56	111.93
1	C	243	TRP	N-CA-CB	5.06	118.43	110.23
1	C	74	ASN	N-CA-C	5.05	119.31	112.04
1	C	59	ASN	O-C-N	-5.04	116.77	123.13
1	C	38	ASP	N-CA-C	5.02	121.50	110.80
1	A	70	ILE	CA-C-O	5.02	126.53	120.66
1	A	5	GLN	CA-C-O	-5.01	115.14	120.40
1	A	97	THR	CB-CA-C	-5.00	100.65	110.11
1	A	237	LYS	CA-C-N	5.00	124.66	119.56
1	A	237	LYS	C-N-CA	5.00	124.66	119.56

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 ⓘ

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	2429	89	0
1	C	2388	0	2430	157	0
2	B	2083	0	2107	62	0
2	D	2083	0	2107	116	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	13	0
4	C	145	0	0	48	0
4	D	83	0	0	11	0
All	All	9765	0	9151	411	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 23.

All (411) 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)
2:B:423:LEU:HB2	4:B:2222:HOH:O	1.63	0.98
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.52	0.91
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
1:C:218:THR:HG22	1:C:219:LEU:HG	1.60	0.82
3:C:1298[A]:6CP:N1	3:C:1298[A]:6CP:H18	1.94	0.82
3:C:1298[B]:6CP:H18	3:C:1298[B]:6CP:N1	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:230:VAL:CG1	1:A:233:MET:HE3	2.15	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
1:A:230:VAL:HA	1:A:233:MET:HE2	1.68	0.76
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
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
2:B:210:MET:HE1	2:B:250:ARG:CB	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
1:A:227:TRP:CZ2	1:A:233:MET:HE1	2.26	0.71
1:C:91:MET:HE2	1:C:196:MET:HA	1.73	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:N1	3:C:1298[A]:6CP:C18	2.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1298[B]:6CP:N1	3:C:1298[B]:6CP:C18	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:H	1:A:74:ASN:ND2	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
2:B:392:MET:HA	2:B:392:MET:HE3	1.78	0.65
1:C:87:LEU:HD23	4:C:2084:HOH:O	1.94	0.65
1:C:133:LEU:HD12	4:C:2084:HOH:O	1.94	0.65
1:A:154:VAL:O	2:B:316:THR:HG23	1.96	0.65
1:C:39:THR:HG22	1:C:40:GLU:H	1.61	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:392:MET:HE2	2:D:392:MET:HA	1.80	0.61
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:A:230:VAL:HA	1:A:233:MET:HE3	1.82	0.61
1:A:230:VAL:HG12	1:A:233:MET:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:ILE:HG22	2:D:210:MET:HE1	1.83	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:91:MET:HE1	4:C:2105:HOH:O	2.02	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:91:MET:HE3	1:C:196:MET:HG3	1.83	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
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
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.40	0.57
2:B:392:MET:HA	2:B:392:MET:CE	2.34	0.57
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.57
1:C:88:LYS:HD3	1:C:131:GLN:NE2	2.20	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:84:HIS:CD2	1:C:296:LEU:HD13	2.42	0.54
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.37	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:51:GLU:O	1:C:55:LEU:HB2	2.07	0.54
1:C:215:ILE:HG23	4:C:2109:HOH:O	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
1:C:91:MET:CE	1:C:196:MET:HG3	2.38	0.53
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.53
1:A:161:HIS:CD2	4:A:2136:HOH:O	2.50	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:C:220:GLY:O	1:C:221:THR:C	2.49	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
2:B:392:MET:HE2	4:B:2197:HOH:O	2.08	0.52
1:C:238:PRO:HB2	4:C:2120:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:131:GLN:CD	1:A:131:GLN:H	2.19	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:A:227:TRP:CE2	1:A:233:MET:HE1	2.45	0.51
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.41	0.51
2:D:206:ILE:HG22	2:D:210:MET:HE2	1.92	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
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:D:338:GLU:CD	2:D:412:LYS:HZ3	2.20	0.50
1:C:217:ARG:HG3	1:C:243:TRP:CD1	2.47	0.50
2:D:334:MET:O	2:D:335:PHE:C	2.55	0.49
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:74:ASN:H	1:A:74:ASN:HD22	1.60	0.49
1:A:91:MET:HE2	1:A:196:MET:HA	1.94	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:35:ILE:HB	1:C:76:LEU:HB3	1.94	0.49
1:C:186:ILE:HG13	1:C:275:ILE:O	2.12	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:A:230:VAL:HG13	1:A:233:MET:HE3	1.93	0.48
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
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:74:ASN:H	1:C:74:ASN:ND2	2.11	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
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:C:295:HIS:ND1	1:C:295:HIS:C	2.70	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.48
1:A:139:GLY:HA2	1:A:293:VAL:HA	1.92	0.48
1:A:223:ASP:H	1:A:226:VAL:CG1	2.27	0.48
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:HG2	2:B:211:ARG:HH11	1.79	0.48
2:D:362:LEU:HD21	2:D:395:HIS:HB2	1.96	0.48
1:A:97:THR:O	1:A:97:THR:HG22	2.14	0.48
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:HG2	2:B:211:ARG:NH1	2.29	0.47
2:D:332:LEU:HD12	2:D:335:PHE:CD2	2.50	0.47
2:D:332:LEU:O	2:D:332:LEU:HG	2.13	0.47
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.83	0.47
1:C:33:LYS:NZ	1:C:51:GLU:OE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:409:ILE:O	2:D:410:ARG:C	2.58	0.46
1:A:39:THR:O	1:A:40:GLU:C	2.58	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:15:TYR:OH	1:C:48:ALA:HA	2.16	0.46
1:C:17:VAL:HB	1:C:19:TYR:CE1	2.51	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46
1:C:100:PRO:O	1:C:104:ILE:HG13	2.16	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:98:GLY:HA2	1:C:199:ARG:NE	2.31	0.45
1:C:156:VAL:HG21	1:C:180:TYR:O	2.16	0.45
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:342:ILE:HG21	2:D:404:HIS:CE1	2.51	0.45
2:D:361:HIS:CD2	2:D:384:LEU:HD11	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
1:C:169:ARG:HG2	1:C:173:ILE:HB	1.97	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:326:ASN:CG	2:D:329:VAL:HG23	2.42	0.45
2:D:402:PRO:HB2	2:D:403:GLN:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:210:MET:HE2	4:B:2104:HOH:O	2.17	0.44
1:A:37:LEU:O	1:A:38:ASP:CB	2.65	0.44
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.99	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:314:PHE:O	2:D:315:LEU:C	2.61	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
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:O	2:D:398:TYR:HD1	2.01	0.43
1:C:39:THR:HG22	1:C:40:GLU:N	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:430:LEU:O	2:B:431:ASN:C	2.62	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:43:GLY:HA3	2:D:292:LEU:HD12	2.01	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
2:D:314:PHE:HA	2:D:317:GLN:HG3	2.02	0.42
1:A:40:GLU:H	2:B:292:LEU:HD23	1.84	0.42
1:A:227:TRP:HB3	1:A:230:VAL:HG22	2.00	0.42
1:A:291:LYS:NZ	4:A:2263:HOH:O	2.44	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:N	2:D:176:PRO:HD3	2.33	0.42
2:D:175:VAL:HG12	2:D:175:VAL:O	2.20	0.42
2:D:230:GLU:O	2:D:231:THR:C	2.63	0.42
1:A:10:ILE:HD13	3:A:1298[A]:6CP:C18	2.50	0.42
2:B:371:SER:O	2:B:372:TRP:C	2.62	0.41
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
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:A:230:VAL:CA	1:A:233:MET:HE3	2.48	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:HE1	2:D:250:ARG:CB	2.51	0.41
2:D:210:MET:O	2:D:213:ILE:HB	2.21	0.41
1:A:261:SER:O	1:A:265:GLN:HG3	2.21	0.41
2:B:428:GLU:H	2:B:428:GLU:HG2	1.56	0.41
1:C:156:VAL:HB	1:C:159:TYR:HE2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ILE:HA	2:D:210:MET:CE	2.51	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.92	0.41
2:D:371:SER:O	2:D:372:TRP:C	2.64	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: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:233:MET:HE2	4:C:2115:HOH:O	2.21	0.40
1:C:72:THR:HG22	1:C:74:ASN:ND2	2.37	0.40
1:C:240:PHE:HD2	4:C:2119:HOH:O	2.02	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%)	6	2
1	C	294/303 (97%)	265 (90%)	18 (6%)	11 (4%)	2	1
2	B	256/258 (99%)	251 (98%)	3 (1%)	2 (1%)	16	11
2	D	256/258 (99%)	230 (90%)	22 (9%)	4 (2%)	7	3
All	All	1100/1122 (98%)	1026 (93%)	51 (5%)	23 (2%)	5	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 ⓘ

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%)	227 (87%)	34 (13%)	4	2
2	B	232/232 (100%)	219 (94%)	13 (6%)	19	16
2	D	232/232 (100%)	206 (89%)	26 (11%)	6	3
All	All	986/994 (99%)	888 (90%)	98 (10%)	7	4

All (98) 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	55	LEU
1	A	72	THR
1	A	73	GLU
1	A	74	ASN
1	A	78	LEU
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	200	MET
2	B	202	LYS
2	B	209	SER
2	B	232	LEU
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

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Mol	Chain	Res	Type
1	C	40	GLU
1	C	41	THR
1	C	57	GLU
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	218	THR
1	C	225	VAL
1	C	226	VAL
1	C	230	VAL
1	C	232	SER
1	C	250	LYS
1	C	255	LEU
1	C	264	SER
1	C	278	LYS
1	C	288	ASP
1	C	296	LEU
2	D	177	ASP
2	D	194	LYS
2	D	197	VAL
2	D	202	LYS
2	D	210	MET
2	D	224	GLU
2	D	232	LEU
2	D	245	SER
2	D	268	GLU
2	D	316	THR
2	D	320	LEU
2	D	324	PRO
2	D	339	LEU

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Mol	Chain	Res	Type
2	D	346	PRO
2	D	349	LYS
2	D	355	ILE
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	417	LYS
2	D	418	TYR
2	D	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) 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	265	GLN
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
2	B	406	GLN
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	85	GLN
1	C	119	HIS
2	D	179	HIS
2	D	233	HIS
2	D	254	GLN

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Mol	Chain	Res	Type
2	D	312	ASN
2	D	313	GLN
2	D	322	GLN
2	D	361	HIS
2	D	395	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	A	160	1	8,10,11	1.63	2 (25%)	10,14,16	1.49	2 (20%)
1	TPO	C	160	1	8,10,11	2.39	2 (25%)	10,14,16	1.65	3 (30%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	4.46	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	4.25	1.67	1.59
1	A	160	TPO	CG2-CB	2.67	1.58	1.51
1	A	160	TPO	P-OG1	2.57	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	P-OG1-CB	-3.19	114.67	123.33
1	A	160	TPO	O-C-CA	-2.95	117.18	124.77
1	A	160	TPO	P-OG1-CB	-2.30	117.06	123.33
1	C	160	TPO	O3P-P-O2P	2.19	116.03	107.80
1	C	160	TPO	O-C-CA	-2.07	119.44	124.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	C-CA-CB-CG2

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 oligosaccharides 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[A]	-	27,28,28	2.44	9 (33%)	34,38,38	2.73	11 (32%)
3	6CP	C	1298[A]	-	27,28,28	2.96	8 (29%)	34,38,38	3.72	15 (44%)
3	6CP	A	1298[B]	-	27,28,28	2.44	9 (33%)	34,38,38	3.11	14 (41%)
3	6CP	C	1298[B]	-	27,28,28	19.10	9 (33%)	34,38,38	12.50	17 (50%)

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298[B]	6CP	C19-CL1	98.05	4.03	1.74
3	C	1298[A]	6CP	C4-N3	8.03	1.45	1.34
3	C	1298[B]	6CP	C4-N3	8.03	1.45	1.34
3	C	1298[A]	6CP	C4-N9	-7.40	1.32	1.38
3	C	1298[B]	6CP	C4-N9	-7.40	1.32	1.38
3	A	1298[A]	6CP	C4-N3	6.85	1.43	1.34
3	A	1298[B]	6CP	C4-N3	6.85	1.43	1.34
3	A	1298[A]	6CP	C4-N9	-5.52	1.33	1.38
3	A	1298[B]	6CP	C4-N9	-5.52	1.33	1.38
3	C	1298[A]	6CP	C6-N1	-5.39	1.24	1.32
3	C	1298[B]	6CP	C6-N1	-5.39	1.24	1.32
3	C	1298[A]	6CP	C2-N1	4.44	1.47	1.34
3	C	1298[B]	6CP	C2-N1	4.44	1.47	1.34
3	A	1298[A]	6CP	C2-N1	4.10	1.46	1.34
3	A	1298[B]	6CP	C2-N1	4.10	1.46	1.34
3	C	1298[A]	6CP	C5-C4	-3.84	1.33	1.40
3	C	1298[B]	6CP	C5-C4	-3.84	1.33	1.40
3	C	1298[A]	6CP	C5-N7	3.71	1.44	1.37
3	C	1298[B]	6CP	C5-N7	3.71	1.44	1.37
3	A	1298[A]	6CP	C5-N7	3.66	1.44	1.37
3	A	1298[B]	6CP	C5-N7	3.66	1.44	1.37
3	A	1298[B]	6CP	C2-N2	-3.08	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298[A]	6CP	C2-N2	-2.92	1.30	1.36
3	A	1298[A]	6CP	C5-C4	-2.85	1.35	1.40
3	A	1298[B]	6CP	C5-C4	-2.85	1.35	1.40
3	A	1298[A]	6CP	C8-N7	-2.65	1.29	1.35
3	A	1298[B]	6CP	C8-N7	-2.65	1.29	1.35
3	C	1298[A]	6CP	C8-N7	-2.64	1.29	1.35
3	C	1298[B]	6CP	C8-N7	-2.64	1.29	1.35
3	A	1298[A]	6CP	C14-C13	2.61	1.61	1.51
3	A	1298[B]	6CP	C14-C13	2.61	1.61	1.51
3	A	1298[B]	6CP	C17-N2	-2.51	1.35	1.40
3	A	1298[A]	6CP	C17-N2	-2.45	1.35	1.40
3	C	1298[A]	6CP	C2-N3	-2.44	1.28	1.34
3	C	1298[B]	6CP	C2-N3	-2.44	1.28	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298[B]	6CP	C20-C19-CL1	-68.34	18.52	119.36
3	C	1298[B]	6CP	C18-C19-CL1	-13.14	102.69	119.17
3	C	1298[A]	6CP	C4-N9-C8	10.84	110.74	103.84
3	C	1298[B]	6CP	C4-N9-C8	10.84	110.74	103.84
3	C	1298[A]	6CP	N3-C4-N9	8.49	132.52	125.68
3	C	1298[B]	6CP	N3-C4-N9	8.49	132.52	125.68
3	A	1298[A]	6CP	C4-N9-C8	7.92	108.88	103.84
3	A	1298[B]	6CP	C4-N9-C8	7.92	108.88	103.84
3	A	1298[A]	6CP	N3-C4-N9	7.63	131.82	125.68
3	A	1298[B]	6CP	N3-C4-N9	7.63	131.82	125.68
3	C	1298[A]	6CP	C2-N1-C6	7.63	128.51	115.38
3	C	1298[B]	6CP	C2-N1-C6	7.63	128.51	115.38
3	C	1298[A]	6CP	N3-C2-N1	-7.47	114.02	126.26
3	C	1298[B]	6CP	N3-C2-N1	-7.47	114.02	126.26
3	A	1298[A]	6CP	C5-C4-N3	-6.33	118.65	124.22
3	A	1298[B]	6CP	C5-C4-N3	-6.33	118.65	124.22
3	C	1298[A]	6CP	O6-C6-N1	6.15	128.24	120.02
3	C	1298[B]	6CP	O6-C6-N1	6.15	128.24	120.02
3	A	1298[B]	6CP	C17-C18-C19	6.03	123.66	118.72
3	A	1298[B]	6CP	C18-C19-CL1	5.57	126.16	119.17
3	C	1298[A]	6CP	C5-C4-N3	-5.51	119.37	124.22
3	C	1298[B]	6CP	C5-C4-N3	-5.51	119.37	124.22
3	A	1298[A]	6CP	N3-C2-N1	-4.68	118.60	126.26
3	A	1298[B]	6CP	N3-C2-N1	-4.68	118.60	126.26
3	C	1298[A]	6CP	N2-C2-N3	4.21	131.36	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298[B]	6CP	N2-C2-N3	4.21	131.36	116.90
3	C	1298[A]	6CP	C17-N2-C2	-3.60	119.67	129.38
3	C	1298[B]	6CP	C17-N2-C2	-3.60	119.67	129.38
3	C	1298[A]	6CP	C21-C22-C17	3.38	123.62	119.73
3	C	1298[B]	6CP	C21-C22-C17	3.38	123.62	119.73
3	C	1298[A]	6CP	C14-C13-C12	3.35	118.30	111.42
3	C	1298[B]	6CP	C14-C13-C12	3.35	118.30	111.42
3	C	1298[A]	6CP	C5-C4-N9	-2.97	108.10	110.46
3	C	1298[B]	6CP	C5-C4-N9	-2.97	108.10	110.46
3	A	1298[B]	6CP	C20-C19-C18	-2.97	117.65	121.53
3	A	1298[A]	6CP	N7-C8-N9	-2.96	109.36	113.87
3	A	1298[B]	6CP	N7-C8-N9	-2.96	109.36	113.87
3	A	1298[A]	6CP	C5-N7-C8	2.89	108.69	106.27
3	A	1298[B]	6CP	C5-N7-C8	2.89	108.69	106.27
3	A	1298[A]	6CP	C2-N1-C6	2.84	120.27	115.38
3	A	1298[B]	6CP	C2-N1-C6	2.84	120.27	115.38
3	C	1298[A]	6CP	C17-C18-C19	2.79	121.00	118.72
3	C	1298[B]	6CP	C17-C18-C19	2.79	121.00	118.72
3	C	1298[A]	6CP	N7-C8-N9	-2.76	109.66	113.87
3	C	1298[B]	6CP	N7-C8-N9	-2.76	109.66	113.87
3	C	1298[A]	6CP	C22-C17-C18	-2.67	116.42	119.66
3	C	1298[B]	6CP	C22-C17-C18	-2.67	116.42	119.66
3	A	1298[A]	6CP	C4-C5-N7	-2.58	103.54	105.28
3	A	1298[B]	6CP	C4-C5-N7	-2.58	103.54	105.28
3	A	1298[A]	6CP	C14-C15-C16	2.47	116.49	111.42
3	A	1298[B]	6CP	C14-C15-C16	2.47	116.49	111.42
3	A	1298[A]	6CP	C21-C22-C17	2.31	122.40	119.73
3	C	1298[A]	6CP	C13-C12-C11	-2.21	107.43	112.08
3	C	1298[B]	6CP	C13-C12-C11	-2.21	107.43	112.08
3	A	1298[B]	6CP	C20-C19-CL1	-2.16	116.17	119.36
3	A	1298[A]	6CP	C13-C12-C11	2.04	116.37	112.08
3	A	1298[B]	6CP	C13-C12-C11	2.04	116.37	112.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

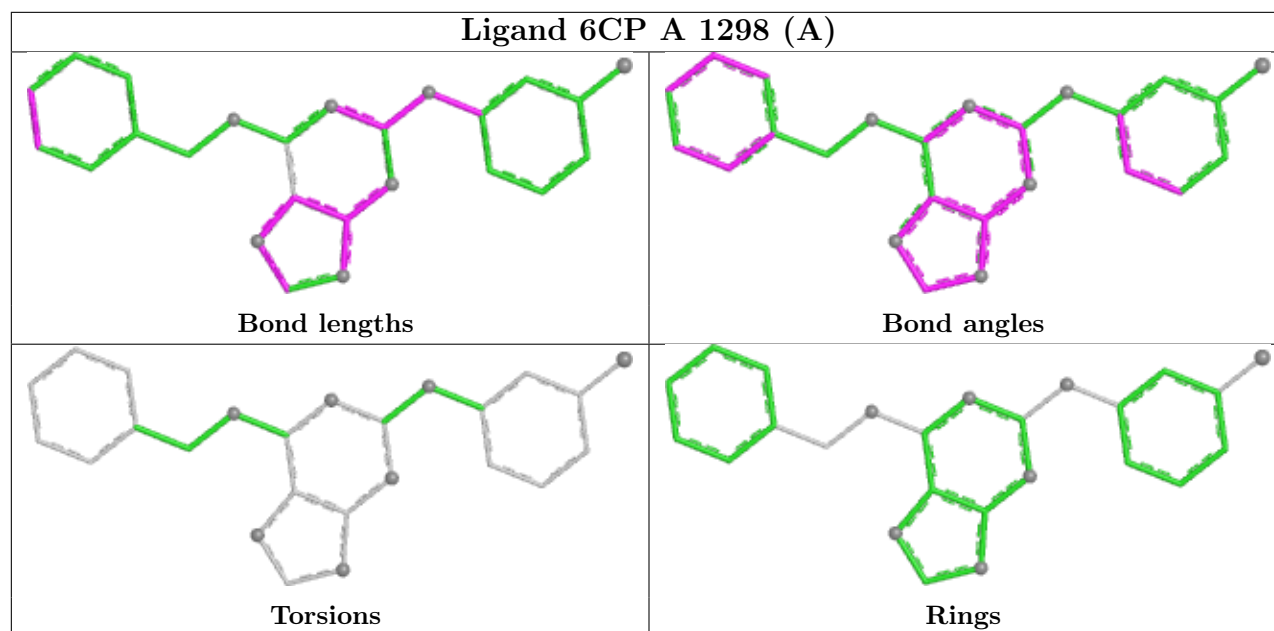
Mol	Chain	Res	Type	Atoms
3	A	1298[B]	6CP	N3-C2-N2-C17
3	A	1298[B]	6CP	N1-C2-N2-C17

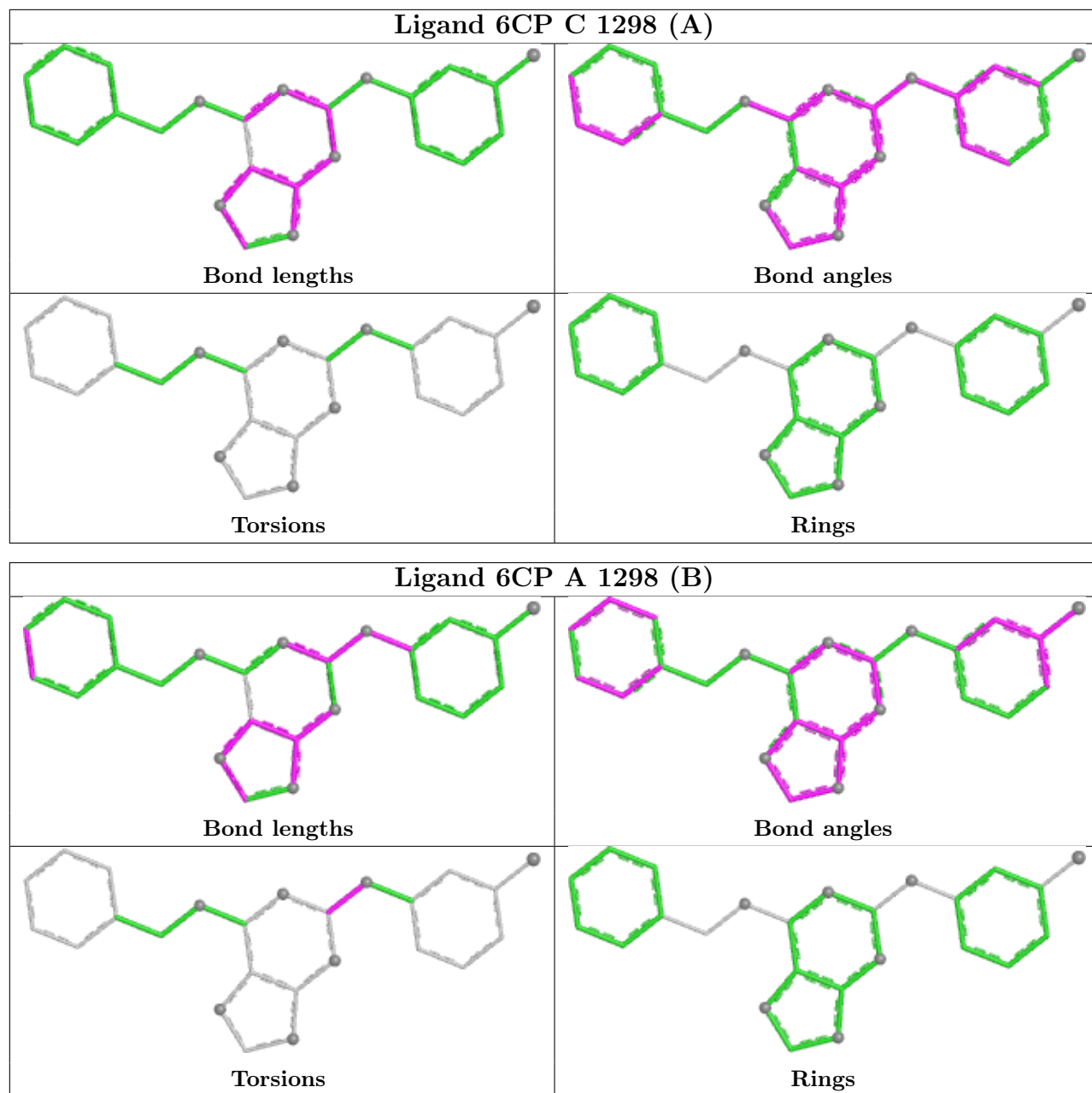
There are no ring outliers.

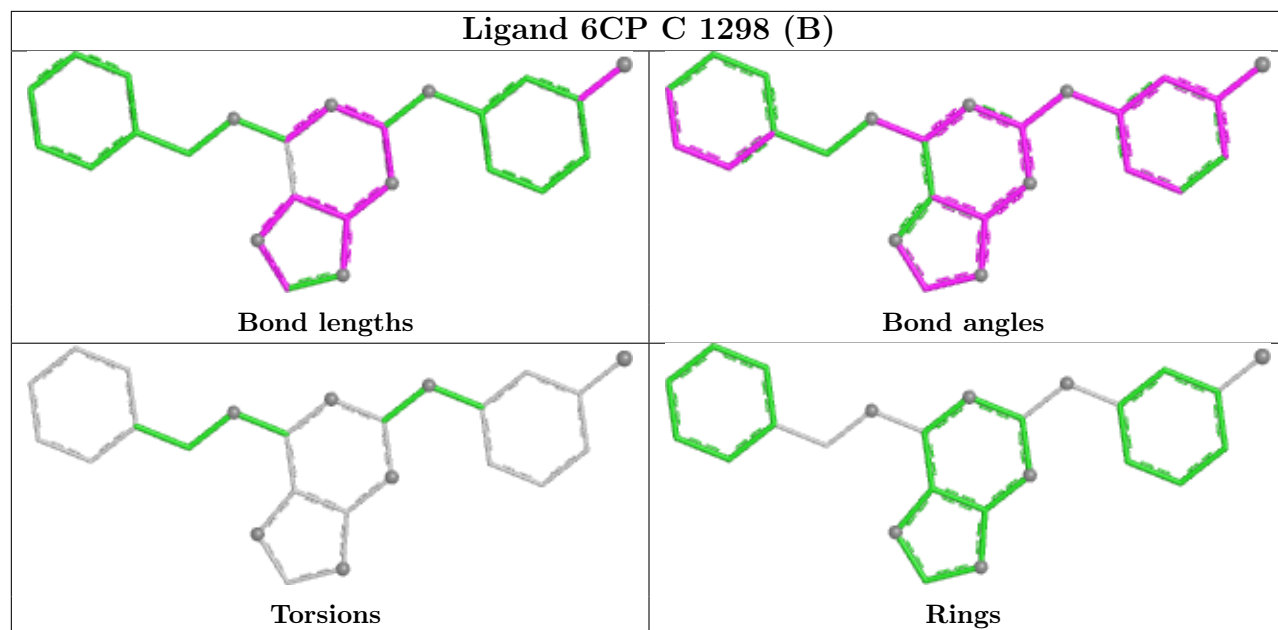
3 monomers are involved in 9 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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%)	0.21	20 (6%) 23 22	19, 31, 61, 91	0
1	C	296/303 (97%)	1.88	108 (36%) 1 1	31, 54, 85, 99	0
2	B	258/258 (100%)	0.01	10 (3%) 43 42	20, 32, 50, 74	0
2	D	258/258 (100%)	1.76	98 (37%) 1 1	31, 58, 85, 96	0
All	All	1108/1122 (98%)	0.97	236 (21%) 2 2	19, 42, 81, 99	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	HIS	10.1
1	A	293	VAL	9.1
1	C	244	ALA	8.9
1	C	230	VAL	8.7
2	B	175	VAL	8.7
1	A	294	PRO	7.9
1	C	241	PRO	7.9
1	C	221	THR	7.4
1	C	39	THR	7.3
1	C	243	TRP	7.0
1	C	236	TYR	6.9
1	C	227	TRP	6.6
1	A	296	LEU	6.4
1	C	233	MET	6.4
1	C	225	VAL	6.4
2	B	423	LEU	6.1
1	C	240	PHE	5.9
1	C	226	VAL	5.8
1	A	96	LEU	5.7
1	C	248	PHE	5.6
1	C	38	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	5.6
2	D	175	VAL	5.5
1	C	40	GLU	5.3
2	D	402	PRO	5.3
1	C	41	THR	5.1
1	C	177	CYS	5.1
1	C	163	VAL	5.1
2	D	364	LEU	5.0
2	D	401	ALA	5.0
2	D	372	TRP	4.9
1	C	251	VAL	4.9
1	C	235	ASP	4.9
1	C	219	LEU	4.9
1	C	222	PRO	4.9
1	C	209	ILE	4.8
1	C	231	THR	4.7
2	D	320	LEU	4.6
2	D	418	TYR	4.6
1	C	242	LYS	4.6
1	A	41	THR	4.5
2	D	429	THR	4.5
1	C	256	ASP	4.4
2	D	360	PHE	4.3
2	D	365	TYR	4.3
1	C	294	PRO	4.3
1	A	71	HIS	4.3
1	C	239	SER	4.3
1	A	72	THR	4.2
2	D	410	ARG	4.2
1	C	217	ARG	4.2
2	D	382	TYR	4.2
1	C	228	PRO	4.2
1	C	253	PRO	4.1
2	D	359	ALA	4.1
1	A	97	THR	4.1
1	C	238	PRO	4.1
2	D	176	PRO	4.1
2	D	430	LEU	4.1
2	D	396	GLN	4.0
1	A	95	ALA	4.0
1	C	216	PHE	3.9
2	D	413	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	279	ALA	3.9
1	C	175	LEU	3.9
2	D	424	LEU	3.9
1	C	165	THR	3.9
1	C	245	ARG	3.8
1	C	271	PRO	3.8
2	D	311	VAL	3.8
1	C	171	PRO	3.8
1	C	234	PRO	3.8
1	C	96	LEU	3.7
2	D	376	LEU	3.7
1	C	72	THR	3.7
2	D	327	CYS	3.7
2	D	432	LEU	3.7
1	C	282	ALA	3.7
2	D	390	CYS	3.6
2	D	367	VAL	3.6
2	D	334	MET	3.6
2	D	384	LEU	3.6
2	D	329	VAL	3.6
1	A	39	THR	3.6
1	C	203	PHE	3.5
1	C	95	ALA	3.5
2	D	383	THR	3.5
2	D	326	ASN	3.5
1	C	269	TYR	3.5
1	C	295	HIS	3.5
2	B	176	PRO	3.5
2	D	362	LEU	3.5
2	D	428	GLU	3.4
1	C	88	LYS	3.4
1	C	156	VAL	3.4
1	C	215	ILE	3.4
2	D	420	GLY	3.4
1	A	38	ASP	3.4
2	D	419	HIS	3.4
2	D	389	PRO	3.4
1	C	296	LEU	3.4
1	C	255	LEU	3.3
2	D	350	TYR	3.3
2	D	363	ALA	3.3
2	D	315	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	427	PRO	3.3
2	D	356	ALA	3.3
2	D	281	ILE	3.3
2	D	332	LEU	3.3
2	D	377	ILE	3.2
1	C	283	HIS	3.2
1	C	246	GLN	3.2
2	D	337	GLY	3.1
2	D	392	MET	3.1
2	B	177	ASP	3.1
2	D	177	ASP	3.1
1	C	104	ILE	3.1
2	B	283	ASP	3.1
1	C	229	GLY	3.1
2	D	373	PRO	3.1
1	C	288	ASP	3.1
1	C	293	VAL	3.1
1	C	286	PHE	3.0
2	D	333	ALA	3.0
2	D	336	LEU	3.0
2	D	387	LEU	3.0
2	D	385	GLU	3.0
2	D	314	PHE	3.0
1	C	71	HIS	3.0
2	D	375	SER	3.0
2	D	319	PHE	3.0
2	D	369	GLY	2.9
2	D	346	PRO	2.9
1	C	199	ARG	2.9
2	D	405	ALA	2.9
2	D	394	LEU	2.9
1	C	223	ASP	2.9
2	D	397	THR	2.9
2	D	325	ALA	2.9
1	C	37	LEU	2.8
2	D	193	CYS	2.8
2	D	371	SER	2.8
2	D	351	LEU	2.8
1	C	252	VAL	2.8
2	D	421	VAL	2.8
1	C	173	ILE	2.8
1	C	212	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	ARG	2.7
1	C	194	ALA	2.7
2	D	380	THR	2.7
1	C	224	GLU	2.7
1	C	264	SER	2.7
2	D	194	LYS	2.7
1	C	153	GLY	2.7
1	C	170	ALA	2.7
1	C	232	SER	2.6
1	C	249	SER	2.6
2	D	284	ASP	2.6
2	D	400	LYS	2.6
2	D	409	ILE	2.6
2	D	403	GLN	2.6
2	D	399	LEU	2.6
2	D	343	ASP	2.6
1	C	220	GLY	2.6
1	C	213	PHE	2.6
1	C	247	ASP	2.6
2	D	431	ASN	2.6
1	C	198	THR	2.6
1	C	262	LEU	2.6
2	D	322	GLN	2.5
2	D	415	ASN	2.5
2	D	426	PRO	2.5
2	D	398	TYR	2.5
2	D	352	PRO	2.5
2	D	358	ALA	2.5
2	D	374	GLU	2.5
1	C	158	THR	2.5
1	C	187	TRP	2.5
2	D	354	VAL	2.4
1	C	204	PRO	2.4
1	C	162	GLU	2.4
1	C	192	ILE	2.4
1	C	191	CYS	2.4
2	D	368	THR	2.4
1	C	237	LYS	2.4
2	D	379	LYS	2.4
2	D	357	GLY	2.4
1	C	210	ASP	2.4
1	C	250	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	97	THR	2.4
1	C	254	PRO	2.4
2	D	178	TYR	2.3
1	C	100	PRO	2.3
2	B	274	GLU	2.3
2	D	370	GLN	2.3
1	C	74	ASN	2.3
2	B	432	LEU	2.3
1	C	59	ASN	2.3
2	D	181	ASP	2.3
1	C	202	LEU	2.3
1	C	172	GLU	2.2
2	D	386	SER	2.2
1	C	164	VAL	2.2
2	D	280	TYR	2.2
1	A	35	ILE	2.2
1	C	2	GLU	2.2
1	A	37	LEU	2.2
1	C	120	SER	2.2
2	D	353	SER	2.2
1	C	176	GLY	2.2
2	B	198	GLY	2.2
1	C	101	LEU	2.2
2	D	227	LEU	2.2
2	D	423	LEU	2.2
1	C	180	TYR	2.2
1	A	138	GLU	2.1
2	D	391	LEU	2.1
1	A	19	TYR	2.1
1	C	292	PRO	2.1
2	D	342	ILE	2.1
2	B	201	LYS	2.1
2	D	416	SER	2.1
1	A	73	GLU	2.0
1	C	174	LEU	2.0
1	C	161	HIS	2.0
1	A	7	VAL	2.0
1	C	261	SER	2.0
2	D	344	ALA	2.0
2	B	431	ASN	2.0
1	C	103	LEU	2.0
2	D	341	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	348	LEU	2.0
1	C	218	THR	2.0
2	D	198	GLY	2.0
1	C	168	TYR	2.0
1	C	179	TYR	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, 95th 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	0.12	34,44,50,52	0
1	TPO	A	160	11/12	0.99	0.05	24,26,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

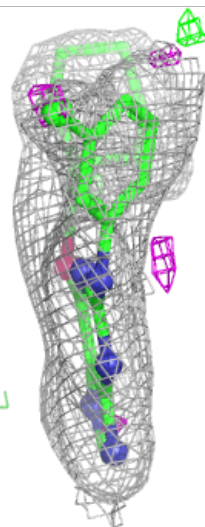
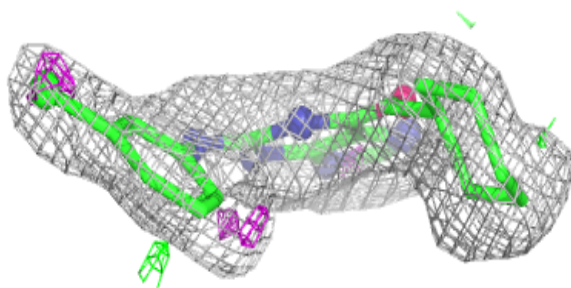
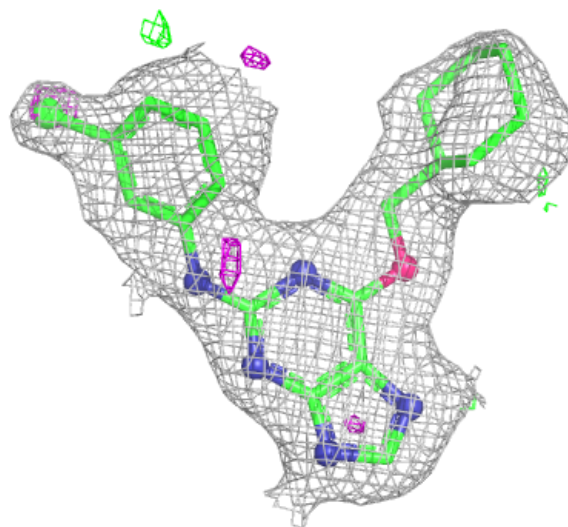
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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[A]	25/25	0.88	0.10	29,35,39,40	25
3	6CP	A	1298[B]	25/25	0.88	0.10	29,34,37,37	25
3	6CP	C	1298[A]	25/25	0.91	0.09	36,42,47,48	25
3	6CP	C	1298[B]	25/25	0.91	0.09	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.

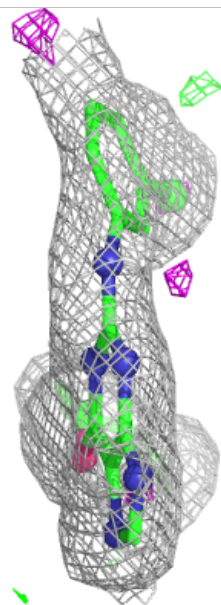
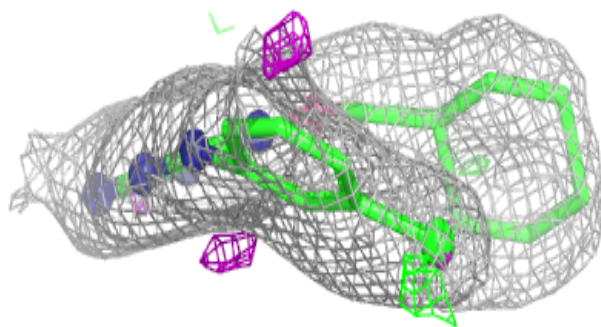
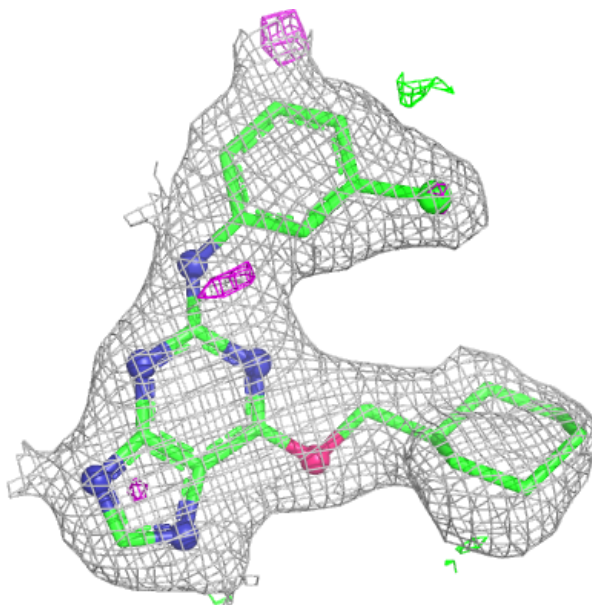
Electron density around 6CP A 1298 (A):

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



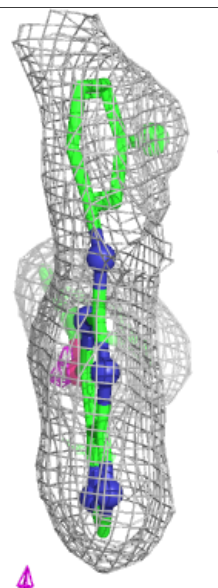
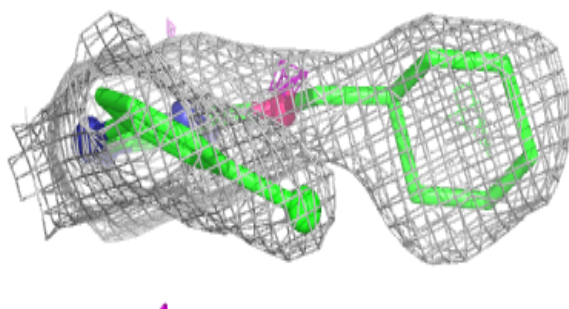
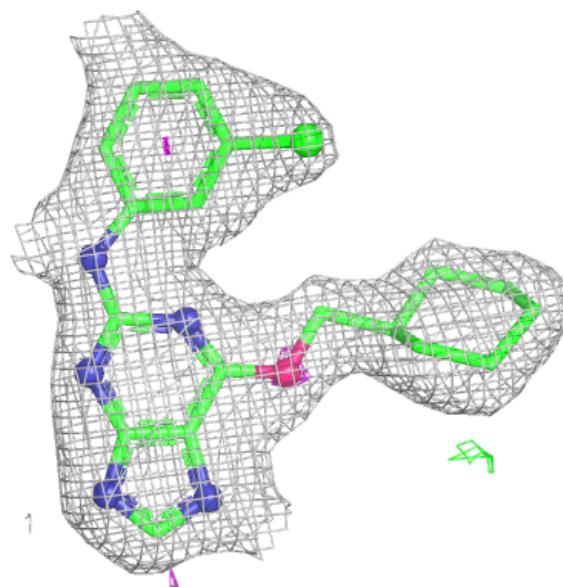
Electron density around 6CP A 1298 (B):

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



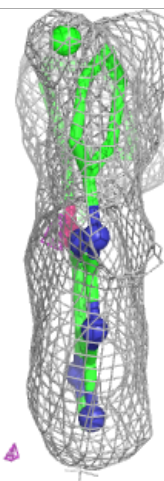
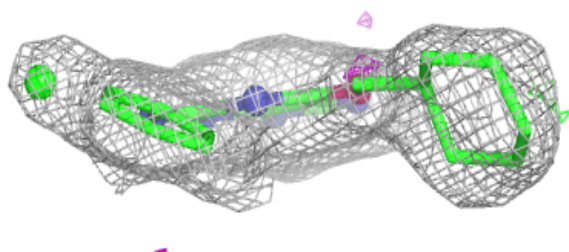
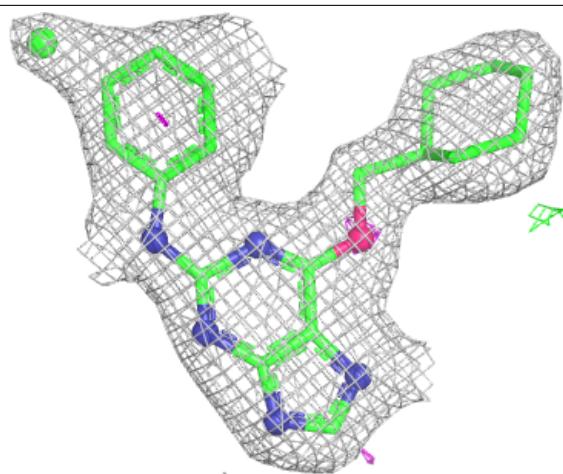
Electron density around 6CP C 1298 (A):

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.