



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 PM UTC

PDB ID : 1CHW / pdb_00001chw
Title : CHALCONE SYNTHASE FROM ALFALFA COMPLEXED WITH
HEXANOYL-COA
Authors : Ferrer, J.-L.; Jez, J.; Bowman, M.E.; Dixon, R.; Noel, J.P.
Deposited on : 1999-03-30
Resolution : 1.90 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

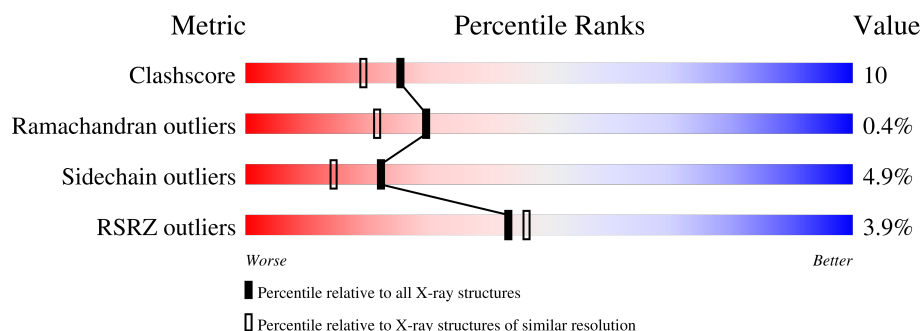
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	389	2% 41% 48% 11%
1	B	389	5% 35% 51% 14%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6636 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.

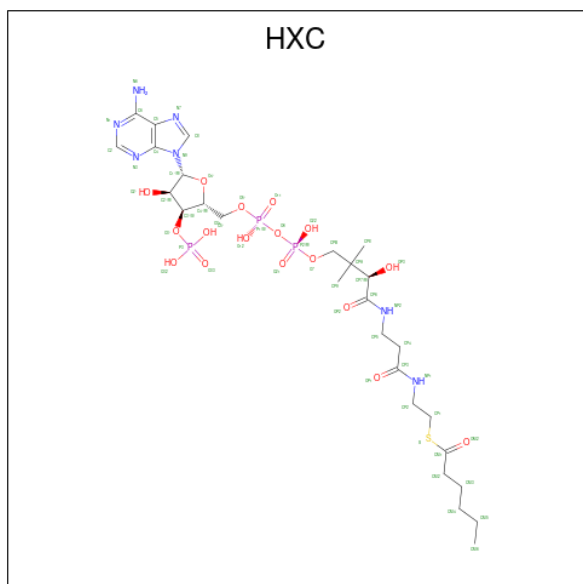
- Molecule 1 is a protein called PROTEIN (CHALCONE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2995	1905	505	566	19			
1	B	389	Total	C	N	O	S	0	0	0
			2995	1905	505	566	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	SER	CYS	engineered mutation	UNP P30074
B	164	SER	CYS	engineered mutation	UNP P30074

- Molecule 2 is HEXANOYL-COENZYME A (CCD ID: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	1
			103	48	14	33	6 2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	1
			103	48	14	33	6	2		

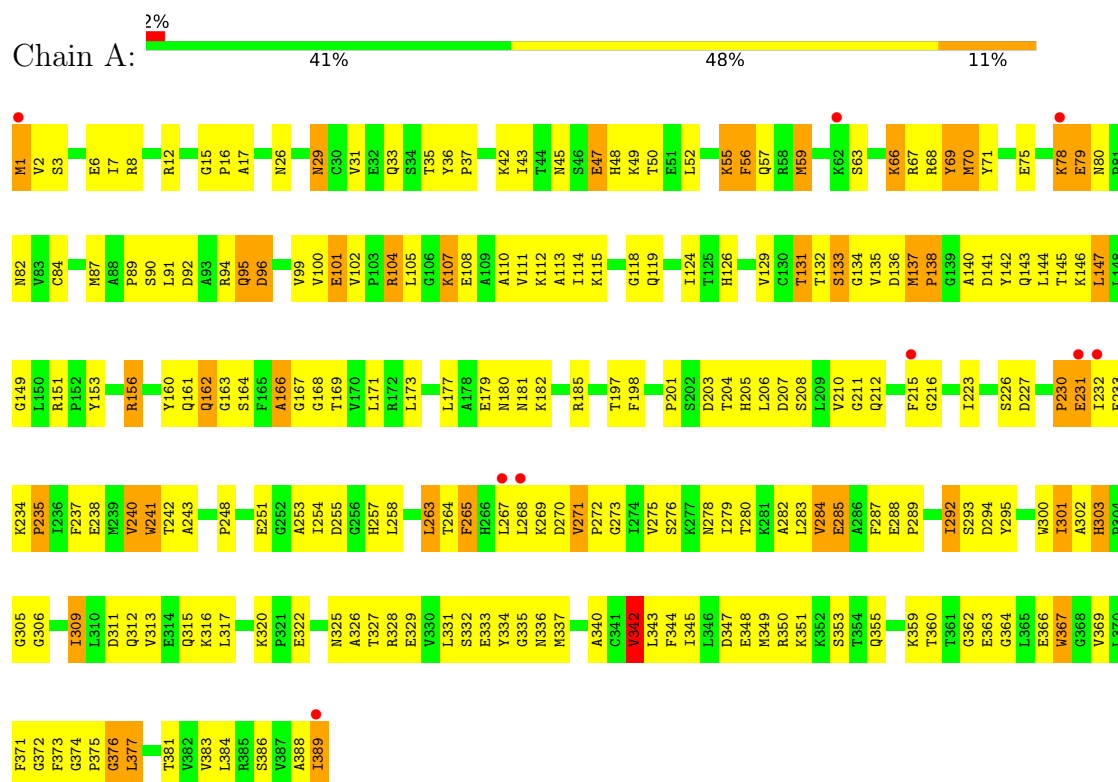
- Molecule 3 is water.

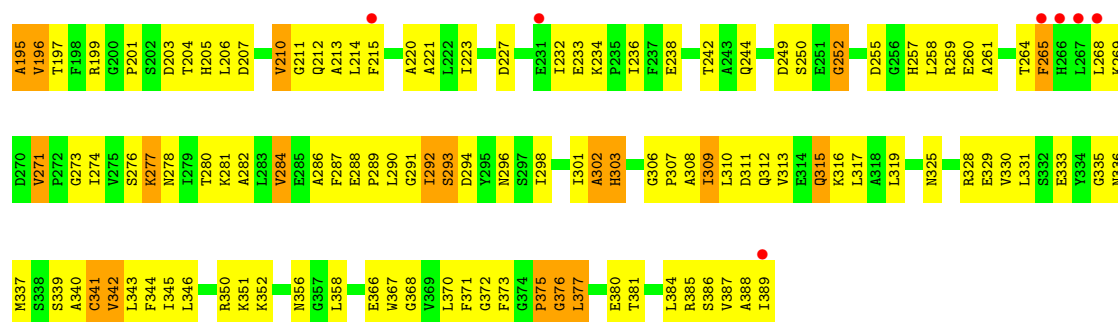
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total	O	0	0
			232	232		
3	B	208	Total	O	0	0
			208	208		

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: PROTEIN (CHALCONE SYNTHASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.81Å 97.81Å 130.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.71 – 1.90 70.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.6 (70.71-1.90) 84.6 (70.71-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.290 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6636	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 93.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1948e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HXC

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	1.14	0/3052	2.73	303/4130 (7.3%)
1	B	1.21	4/3052 (0.1%)	2.96	354/4130 (8.6%)
All	All	1.18	4/6104 (0.1%)	2.85	657/8260 (8.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	10
All	All	0	19

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	THR	CB-OG1	7.03	1.55	1.43
1	B	368	GLY	N-CA	5.78	1.50	1.45
1	B	126	HIS	CG-CD2	5.46	1.41	1.35
1	B	376	GLY	C-O	5.01	1.30	1.23

All (657) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	GLY	O-C-N	-20.07	96.61	122.70
1	A	376	GLY	O-C-N	-16.44	101.33	122.70
1	B	137	MET	CA-C-O	-16.39	100.39	120.23
1	B	168	GLY	O-C-N	-13.99	108.62	122.19
1	B	92	ASP	CA-C-O	-13.73	106.40	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ASN	OD1-CG-ND2	13.62	136.22	122.60
1	B	172	ARG	NE-CZ-NH2	13.62	131.45	119.20
1	B	388	ALA	CA-C-N	13.18	145.43	121.70
1	B	388	ALA	C-N-CA	13.18	145.43	121.70
1	B	142	TYR	CA-C-O	-12.96	107.21	120.82
1	B	336	ASN	OD1-CG-ND2	-12.95	109.65	122.60
1	A	137	MET	CA-C-O	-12.26	105.39	120.23
1	B	41	PHE	CA-CB-CG	-11.84	101.96	113.80
1	B	319	LEU	CA-C-O	-11.78	108.72	121.56
1	A	26	ASN	O-C-N	11.78	129.25	121.71
1	B	33	GLN	OE1-CD-NE2	-11.55	111.05	122.60
1	A	240	VAL	CA-C-O	-11.16	110.18	120.34
1	A	12	ARG	NE-CZ-NH2	-11.12	109.19	119.20
1	B	112	LYS	CA-C-O	11.12	132.50	120.82
1	B	317	LEU	CA-C-O	-11.08	106.00	119.18
1	B	68	ARG	NE-CZ-NH2	11.00	129.10	119.20
1	B	82	ASN	OD1-CG-ND2	-10.89	111.71	122.60
1	B	175	LYS	CA-C-O	10.75	132.90	121.07
1	A	282	ALA	CA-C-O	10.74	131.93	120.55
1	A	273	GLY	CA-C-O	-10.70	108.64	120.09
1	B	119	GLN	OE1-CD-NE2	10.67	133.27	122.60
1	A	67	ARG	NE-CZ-NH1	10.64	132.14	121.50
1	A	336	ASN	OD1-CG-ND2	10.55	133.15	122.60
1	B	385	ARG	CA-C-O	-10.53	109.21	121.11
1	A	313	VAL	CA-C-O	10.49	131.97	120.85
1	B	232	ILE	CA-C-O	10.31	129.97	120.80
1	B	143	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	B	56	PHE	CA-C-O	-10.25	109.68	120.55
1	A	181	ASN	OD1-CG-ND2	10.13	132.73	122.60
1	B	168	GLY	CA-C-O	10.11	131.38	120.66
1	A	331	LEU	CA-C-O	10.07	131.22	120.55
1	B	185	ARG	NE-CZ-NH2	10.05	128.25	119.20
1	A	353	SER	CA-C-N	10.04	134.09	120.44
1	A	353	SER	C-N-CA	10.04	134.09	120.44
1	B	315	GLN	O-C-N	-10.02	111.75	122.07
1	B	65	ILE	CA-C-O	-9.99	109.33	120.72
1	A	303	HIS	CA-CB-CG	-9.96	103.83	113.80
1	A	29	ASN	CA-C-O	9.93	132.43	120.62
1	A	179	GLU	CA-C-O	-9.90	110.05	120.55
1	B	86	TYR	CA-C-O	9.89	130.90	120.42
1	A	56	PHE	CA-C-O	9.88	131.19	120.82
1	A	388	ALA	CA-C-O	9.87	132.16	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	VAL	CA-C-O	9.86	131.21	120.95
1	A	138	PRO	N-CA-CB	9.85	113.59	103.25
1	B	329	GLU	CA-C-O	9.84	130.98	120.55
1	B	206	LEU	CA-C-O	9.82	131.27	119.97
1	A	33	GLN	OE1-CD-NE2	9.81	132.41	122.60
1	B	105	LEU	CA-C-O	9.80	130.81	120.42
1	B	114	ILE	CA-C-O	-9.78	110.49	120.85
1	B	312	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	B	244	GLN	CG-CD-NE2	9.74	131.01	116.40
1	A	334	TYR	O-C-N	9.68	132.37	122.10
1	A	232	ILE	N-CA-C	-9.57	103.33	111.56
1	B	286	ALA	CA-C-O	-9.54	110.35	120.55
1	B	92	ASP	O-C-N	9.49	131.84	122.07
1	B	83	VAL	CA-C-O	-9.47	110.24	120.47
1	A	376	GLY	N-CA-C	-9.45	90.78	113.18
1	B	167	GLY	N-CA-C	-9.43	99.71	113.86
1	A	12	ARG	CD-NE-CZ	9.43	137.60	124.40
1	B	11	GLN	OE1-CD-NE2	-9.40	113.20	122.60
1	B	67	ARG	NE-CZ-NH2	-9.37	110.76	119.20
1	B	280	THR	CA-C-O	9.37	130.48	120.55
1	A	212	GLN	CA-C-O	9.35	130.33	120.42
1	B	182	LYS	CA-C-O	-9.33	110.29	120.92
1	A	284	VAL	CA-C-O	-9.31	110.42	120.47
1	A	227	ASP	CA-C-O	9.30	132.91	120.16
1	B	376	GLY	CA-C-O	-9.30	104.39	120.57
1	A	373	PHE	CA-C-O	-9.26	110.02	120.66
1	A	180	ASN	OD1-CG-ND2	9.21	131.81	122.60
1	B	80	ASN	CB-CG-ND2	9.17	130.15	116.40
1	B	170	VAL	CA-C-O	-9.17	110.57	120.47
1	B	8	ARG	NH1-CZ-NH2	9.10	131.13	119.30
1	B	30	CYS	CA-C-O	9.09	130.61	120.43
1	B	236	ILE	CA-C-O	9.08	128.83	120.30
1	B	278	ASN	CB-CG-ND2	9.07	130.01	116.40
1	B	372	GLY	CA-C-O	-9.05	111.77	120.64
1	B	315	GLN	CA-C-O	8.93	130.20	120.82
1	A	143	GLN	OE1-CD-NE2	8.93	131.53	122.60
1	A	366	GLU	CA-C-O	-8.92	111.43	120.80
1	B	161	GLN	OE1-CD-NE2	8.91	131.51	122.60
1	A	359	LYS	CA-C-O	-8.89	109.30	119.79
1	B	162	GLN	OE1-CD-NE2	-8.89	113.71	122.60
1	B	317	LEU	O-C-N	8.87	135.01	122.41
1	B	212	GLN	OE1-CD-NE2	-8.86	113.74	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	VAL	N-CA-CB	-8.82	95.56	110.65
1	B	14	GLU	CA-C-O	-8.81	108.17	120.07
1	A	334	TYR	CA-C-O	-8.80	108.51	118.55
1	B	207	ASP	CA-CB-CG	8.80	121.40	112.60
1	B	178	ALA	CA-C-O	8.80	129.75	120.42
1	A	173	LEU	CA-C-O	8.75	130.19	121.00
1	A	107	LYS	CA-C-O	8.73	129.80	120.55
1	B	343	LEU	CA-C-O	-8.67	111.23	120.42
1	A	327	THR	CA-C-O	8.65	129.91	120.82
1	B	335	GLY	O-C-N	-8.60	114.73	122.90
1	B	34	SER	CA-C-O	-8.59	111.70	120.90
1	B	38	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	168	GLY	CA-C-O	-8.56	111.31	120.90
1	A	133	SER	CA-C-O	-8.55	111.15	120.30
1	A	114	ILE	CA-C-O	8.53	129.82	120.95
1	B	41	PHE	CA-C-O	-8.45	111.59	120.55
1	A	388	ALA	N-CA-CB	8.39	122.34	109.85
1	B	259	ARG	NH1-CZ-NH2	-8.35	108.44	119.30
1	A	12	ARG	NH1-CZ-NH2	8.35	130.15	119.30
1	A	241	TRP	CA-C-O	-8.34	111.64	120.99
1	A	63	SER	CA-C-O	8.32	129.56	119.49
1	B	142	TYR	O-C-N	8.30	130.62	122.07
1	B	180	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	A	251	GLU	CA-C-O	8.29	130.37	120.92
1	A	99	VAL	CA-C-O	8.24	130.07	119.85
1	B	116	GLU	CA-C-O	8.21	129.44	120.82
1	B	12	ARG	CA-C-O	-8.20	111.65	121.66
1	A	111	VAL	O-C-N	-8.20	113.92	121.87
1	B	214	LEU	N-CA-C	8.18	123.86	113.55
1	B	276	SER	CA-C-O	8.15	129.19	120.55
1	A	265	PHE	CA-CB-CG	8.14	121.94	113.80
1	A	389	ILE	CA-CB-CG2	8.13	124.33	110.50
1	B	341	CYS	CA-C-O	8.13	129.60	120.90
1	A	325	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	B	342	VAL	CB-CA-C	8.10	124.72	112.16
1	B	175	LYS	O-C-N	-8.10	113.41	122.08
1	A	315	GLN	CA-C-O	-8.09	112.36	120.70
1	B	68	ARG	NE-CZ-NH1	-8.07	113.43	121.50
1	A	215	PHE	CA-CB-CG	8.01	121.81	113.80
1	A	287	PHE	CA-CB-CG	-7.98	105.82	113.80
1	B	265	PHE	O-C-N	-7.98	113.85	123.19
1	A	316	LYS	CA-C-O	7.97	129.43	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	LEU	O-C-N	-7.95	113.72	122.79
1	A	328	ARG	NH1-CZ-NH2	7.95	129.63	119.30
1	B	77	LEU	CA-C-O	-7.95	111.12	120.10
1	B	301	ILE	CA-C-O	-7.93	112.26	120.27
1	A	326	ALA	CA-C-O	-7.90	112.05	120.42
1	B	101	GLU	CA-C-O	7.89	128.79	120.42
1	B	249	ASP	CA-C-O	-7.88	112.40	121.54
1	A	226	SER	O-C-N	-7.87	114.14	123.03
1	A	311	ASP	CA-C-O	-7.86	112.09	120.42
1	B	65	ILE	O-C-N	7.85	131.15	123.14
1	B	333	GLU	CA-C-O	7.85	128.46	119.27
1	B	58	ARG	CA-C-O	7.83	129.04	120.82
1	B	158	MET	CA-C-O	-7.82	111.99	120.36
1	B	278	ASN	OD1-CG-ND2	-7.82	114.78	122.60
1	B	325	ASN	O-C-N	-7.81	114.03	122.07
1	B	195	ALA	CA-C-O	7.80	128.91	120.10
1	B	310	LEU	CA-C-O	-7.74	112.69	120.82
1	A	141	ASP	CA-C-N	7.74	130.96	120.44
1	A	141	ASP	C-N-CA	7.74	130.96	120.44
1	B	8	ARG	NE-CZ-NH2	-7.74	112.24	119.20
1	A	374	GLY	O-C-N	7.73	129.50	121.77
1	B	99	VAL	CA-C-O	-7.70	110.71	120.03
1	B	193	VAL	O-C-N	-7.70	114.94	123.26
1	A	285	GLU	CA-C-O	7.70	128.71	120.55
1	B	258	LEU	CA-C-O	-7.69	111.57	120.49
1	A	182	LYS	CA-C-O	7.67	129.32	120.96
1	B	109	ALA	CA-C-O	7.66	128.86	120.82
1	B	287	PHE	CA-C-O	7.63	127.14	118.97
1	B	284	VAL	CA-CB-CG1	7.62	123.35	110.40
1	B	232	ILE	O-C-N	-7.61	116.12	121.98
1	B	273	GLY	CA-C-O	7.61	128.67	120.30
1	B	75	GLU	CA-C-O	7.59	128.60	120.55
1	B	172	ARG	O-C-N	-7.56	114.22	122.09
1	B	128	ILE	O-C-N	7.56	131.12	123.18
1	A	113	ALA	CA-C-O	-7.54	112.83	120.90
1	B	346	LEU	O-C-N	7.53	130.10	122.12
1	A	171	LEU	O-C-N	7.52	130.72	122.15
1	B	271	VAL	CA-C-O	-7.51	109.88	119.95
1	B	139	GLY	CA-C-O	-7.50	111.93	122.51
1	B	86	TYR	CA-CB-CG	-7.48	100.44	113.90
1	A	303	HIS	CA-C-O	7.46	126.82	119.51
1	B	367	TRP	CA-C-N	-7.45	113.58	121.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	TRP	C-N-CA	-7.45	113.58	121.48
1	B	199	ARG	O-C-N	7.45	131.66	123.10
1	B	220	ALA	O-C-N	-7.43	114.20	123.27
1	B	45	ASN	CB-CG-ND2	-7.38	105.33	116.40
1	A	381	THR	O-C-N	-7.36	114.61	123.29
1	A	309	ILE	CA-C-O	7.34	128.95	121.17
1	A	162	GLN	CA-C-O	7.34	128.40	120.55
1	A	383	VAL	N-CA-CB	7.33	119.79	110.99
1	B	74	GLU	CA-C-O	-7.33	112.78	120.55
1	B	104	ARG	NE-CZ-NH2	-7.33	112.61	119.20
1	B	227	ASP	O-C-N	7.32	124.90	121.53
1	A	253	ALA	N-CA-CB	7.29	120.59	110.01
1	B	259	ARG	CD-NE-CZ	7.28	134.60	124.40
1	A	94	ARG	CA-C-N	7.28	129.90	120.44
1	A	94	ARG	C-N-CA	7.28	129.90	120.44
1	A	278	ASN	OD1-CG-ND2	7.25	129.85	122.60
1	A	47	GLU	CA-C-O	-7.25	110.71	119.49
1	A	107	LYS	O-C-N	-7.25	114.44	122.12
1	A	381	THR	CA-C-O	7.24	128.27	120.38
1	B	273	GLY	O-C-N	-7.21	114.42	122.28
1	B	250	SER	CA-C-O	7.21	128.14	119.78
1	A	322	GLU	CA-C-O	-7.20	110.53	119.38
1	A	351	LYS	O-C-N	-7.19	114.50	122.12
1	A	289	PRO	CA-C-O	7.19	129.06	119.00
1	B	306	GLY	O-C-N	7.18	128.95	121.77
1	A	231	GLU	CA-C-N	7.16	130.31	123.08
1	A	231	GLU	C-N-CA	7.16	130.31	123.08
1	B	154	VAL	O-C-N	-7.15	115.06	122.63
1	A	26	ASN	CB-CG-ND2	7.13	127.10	116.40
1	A	15	GLY	CA-C-N	7.13	127.10	119.76
1	A	15	GLY	C-N-CA	7.13	127.10	119.76
1	A	105	LEU	CA-C-O	-7.12	111.78	119.97
1	B	199	ARG	CA-C-O	-7.11	113.84	121.45
1	B	337	MET	CA-C-O	7.10	129.31	119.80
1	A	325	ASN	N-CA-C	7.10	118.67	111.07
1	B	291	GLY	CA-C-N	-7.09	114.39	123.19
1	B	291	GLY	C-N-CA	-7.09	114.39	123.19
1	B	128	ILE	CA-C-N	-7.08	113.86	123.14
1	B	128	ILE	C-N-CA	-7.08	113.86	123.14
1	A	283	LEU	CA-C-O	-7.08	113.38	120.82
1	B	302	ALA	CA-C-N	-7.08	111.03	120.65
1	B	302	ALA	C-N-CA	-7.08	111.03	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	A	386	SER	CA-C-O	7.06	129.43	122.01
1	A	177	LEU	CA-C-O	7.04	128.02	120.55
1	A	292	ILE	CA-CB-CG2	7.04	122.47	110.50
1	A	84	CYS	CA-C-O	-7.03	110.11	119.11
1	A	171	LEU	CA-C-O	-7.03	112.97	120.42
1	A	173	LEU	O-C-N	-7.03	114.72	122.03
1	A	57	GLN	OE1-CD-NE2	-7.02	115.58	122.60
1	B	12	ARG	N-CA-CB	-7.02	99.61	110.56
1	A	138	PRO	CA-N-CD	-7.00	102.21	112.00
1	B	39	PHE	CA-CB-CG	6.97	120.77	113.80
1	A	31	VAL	CA-C-O	6.94	128.16	120.59
1	A	329	GLU	CA-C-O	-6.94	113.07	120.42
1	A	333	GLU	CA-C-O	-6.90	110.75	119.31
1	B	319	LEU	O-C-N	6.89	130.99	122.86
1	A	302	ALA	CA-C-O	-6.88	112.69	120.32
1	B	380	GLU	O-C-N	6.88	131.41	123.29
1	A	16	PRO	CA-C-O	-6.87	113.50	121.34
1	A	237	PHE	CA-C-O	-6.87	113.10	121.06
1	A	216	GLY	O-C-N	-6.86	117.63	123.60
1	B	173	LEU	CA-C-O	-6.86	110.69	120.51
1	B	211	GLY	CA-C-N	6.86	130.16	120.28
1	B	211	GLY	C-N-CA	6.86	130.16	120.28
1	B	190	CYS	O-C-N	6.86	131.02	123.27
1	A	342	VAL	CG1-CB-CG2	6.84	125.86	110.80
1	B	107	LYS	O-C-N	6.84	129.37	122.12
1	A	377	LEU	N-CA-CB	6.83	121.64	110.17
1	B	36	TYR	CA-C-O	6.83	125.42	118.73
1	B	306	GLY	CA-C-O	-6.82	111.77	121.52
1	A	156	ARG	NH1-CZ-NH2	6.81	128.15	119.30
1	B	59	MET	CA-C-O	-6.80	113.67	120.82
1	B	85	GLU	O-C-N	-6.79	115.11	122.85
1	A	342	VAL	N-CA-CB	-6.79	98.48	110.77
1	B	345	ILE	N-CA-C	6.77	116.92	110.42
1	A	145	THR	CA-CB-OG1	-6.77	99.44	109.60
1	B	141	ASP	OD1-CG-OD2	-6.75	106.69	122.90
1	A	67	ARG	O-C-N	6.74	130.34	123.26
1	A	143	GLN	CA-C-O	6.74	127.69	120.55
1	B	135	VAL	O-C-N	-6.72	115.34	123.00
1	A	280	THR	CA-C-O	-6.71	113.79	120.70
1	A	100	VAL	CA-C-O	6.70	127.73	120.69
1	A	212	GLN	O-C-N	-6.69	114.52	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ILE	N-CA-CB	6.69	120.35	111.25
1	A	295	TYR	CA-C-O	6.67	127.12	119.18
1	A	328	ARG	CA-C-O	6.67	127.62	120.55
1	B	189	VAL	CA-C-O	-6.67	113.77	120.31
1	A	198	PHE	CA-C-O	-6.67	113.69	120.96
1	A	306	GLY	O-C-N	-6.66	115.11	121.77
1	B	168	GLY	CA-C-N	6.63	129.17	120.28
1	B	168	GLY	C-N-CA	6.63	129.17	120.28
1	A	137	MET	CB-CA-C	6.62	119.74	109.15
1	B	74	GLU	CA-C-N	6.61	129.14	120.28
1	B	74	GLU	C-N-CA	6.61	129.14	120.28
1	B	309	ILE	CB-CA-C	-6.61	103.52	111.97
1	B	252	GLY	CA-C-O	-6.60	111.08	119.13
1	B	55	LYS	CB-CA-C	-6.58	100.54	110.88
1	A	26	ASN	CA-C-O	-6.58	114.45	120.50
1	B	308	ALA	CA-C-O	6.58	127.53	119.97
1	A	316	LYS	O-C-N	-6.57	115.25	122.09
1	A	185	ARG	NE-CZ-NH1	6.57	128.06	121.50
1	B	96	ASP	CA-C-O	-6.54	113.56	120.63
1	B	260	GLU	CA-C-O	-6.54	112.71	120.10
1	B	75	GLU	CB-CG-CD	6.54	123.71	112.60
1	A	328	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	233	GLU	CA-C-O	-6.53	113.57	121.28
1	A	208	SER	CA-C-O	6.53	127.48	120.10
1	B	146	LYS	CA-C-O	-6.52	113.98	120.70
1	B	352	LYS	CA-C-O	6.50	127.31	120.42
1	B	137	MET	O-C-N	6.49	128.08	121.72
1	B	171	LEU	CA-C-O	6.49	127.39	120.70
1	A	156	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	A	145	THR	CA-C-N	6.46	129.22	120.44
1	A	145	THR	C-N-CA	6.46	129.22	120.44
1	B	72	LEU	CA-C-O	-6.46	113.09	120.58
1	A	282	ALA	O-C-N	-6.45	115.29	122.12
1	A	95	GLN	O-C-N	-6.43	115.44	122.07
1	A	384	LEU	CA-C-N	-6.43	113.93	122.99
1	A	384	LEU	C-N-CA	-6.43	113.93	122.99
1	B	146	LYS	O-C-N	6.42	129.02	122.09
1	B	234	LYS	CA-C-O	6.42	127.39	120.08
1	A	257	HIS	CA-C-O	-6.40	113.45	120.36
1	B	8	ARG	CA-C-O	-6.40	113.64	120.42
1	B	35	THR	CA-C-O	6.40	127.03	119.28
1	A	151	ARG	O-C-N	6.39	128.59	121.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	VAL	CA-CB-CG2	6.38	121.25	110.40
1	A	278	ASN	CA-C-O	6.38	126.81	119.35
1	A	68	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	A	243	ALA	CA-C-O	-6.36	113.87	120.99
1	B	325	ASN	OD1-CG-ND2	6.35	128.95	122.60
1	A	67	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	B	330	VAL	O-C-N	6.35	128.37	121.83
1	B	70	MET	CA-C-O	6.34	128.77	120.21
1	B	18	THR	CA-C-O	-6.34	113.86	120.70
1	A	126	HIS	O-C-N	-6.34	115.54	123.27
1	A	287	PHE	N-CA-C	6.34	121.29	113.50
1	B	366	GLU	CB-CA-C	-6.31	101.17	110.95
1	B	81	PRO	O-C-N	-6.31	114.08	122.22
1	B	138	PRO	N-CA-CB	6.31	109.54	102.60
1	A	79	GLU	CB-CA-C	-6.29	98.68	110.01
1	B	58	ARG	O-C-N	-6.29	115.59	122.07
1	B	387	VAL	O-C-N	6.29	129.83	123.10
1	B	49	LYS	CA-C-N	6.29	129.03	120.54
1	B	49	LYS	C-N-CA	6.29	129.03	120.54
1	B	185	ARG	CB-CA-C	6.27	120.17	110.14
1	B	54	GLU	CB-CG-CD	6.26	123.25	112.60
1	A	144	LEU	CA-C-O	-6.26	112.77	119.97
1	B	316	LYS	CA-C-O	6.25	127.18	120.55
1	B	346	LEU	CA-C-O	-6.25	113.93	120.55
1	A	335	GLY	CA-C-O	-6.25	114.66	122.65
1	A	311	ASP	O-C-N	6.24	129.26	122.15
1	B	80	ASN	O-C-N	-6.24	115.79	121.34
1	B	331	LEU	CA-C-O	-6.24	113.94	120.55
1	B	384	LEU	CA-C-O	-6.23	114.17	121.46
1	A	284	VAL	N-CA-CB	6.23	122.05	110.77
1	A	48	HIS	CA-CB-CG	6.22	120.02	113.80
1	A	312	GLN	OE1-CD-NE2	6.21	128.81	122.60
1	A	349	MET	CA-C-O	-6.21	114.31	120.82
1	B	126	HIS	O-C-N	6.20	130.46	123.27
1	B	149	GLY	CA-C-O	6.19	127.13	119.88
1	A	167	GLY	N-CA-C	-6.19	104.85	112.77
1	A	131	THR	CA-C-O	-6.18	114.09	120.89
1	A	149	GLY	CA-C-O	-6.18	112.77	119.82
1	A	223	ILE	CA-C-O	-6.18	113.96	120.39
1	B	288	GLU	N-CA-CB	6.17	120.00	110.43
1	A	309	ILE	N-CA-C	-6.17	104.50	110.42
1	A	69	TYR	CA-CB-CG	-6.15	102.83	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	THR	O-C-N	-6.15	115.98	123.30
1	B	164	SER	CA-C-O	6.14	126.97	119.11
1	A	49	LYS	O-C-N	-6.14	114.51	122.56
1	B	156	ARG	N-CA-C	6.13	119.47	109.59
1	A	240	VAL	O-C-N	6.13	128.22	121.97
1	A	92	ASP	OD1-CG-OD2	6.13	137.61	122.90
1	B	103	PRO	CA-C-O	-6.13	110.33	119.34
1	A	161	GLN	CA-C-O	6.13	128.65	121.54
1	A	205	HIS	CA-C-O	6.12	131.57	122.32
1	B	274	ILE	O-C-N	6.12	128.14	121.83
1	B	277	LYS	CB-CA-C	-6.12	98.92	110.67
1	A	267	LEU	CA-C-O	-6.12	113.73	120.70
1	A	114	ILE	O-C-N	-6.09	115.96	121.87
1	B	375	PRO	CA-C-O	6.08	127.95	121.32
1	A	142	TYR	N-CA-C	-6.08	104.57	111.14
1	B	156	ARG	O-C-N	-6.08	115.49	123.21
1	B	313	VAL	O-C-N	6.07	128.08	121.83
1	B	79	GLU	CA-C-O	6.06	126.87	119.11
1	A	347	ASP	O-C-N	-6.05	115.83	122.07
1	A	271	VAL	O-C-N	-6.05	114.20	121.10
1	B	80	ASN	N-CA-C	6.04	119.58	108.94
1	A	67	ARG	CA-C-O	-6.04	114.98	121.38
1	A	80	ASN	CA-CB-CG	6.04	118.64	112.60
1	A	181	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	326	ALA	O-C-N	6.04	129.04	122.15
1	A	162	GLN	CB-CG-CD	6.02	122.84	112.60
1	A	344	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	197	THR	CA-C-O	-6.01	112.52	119.14
1	B	40	TYR	N-CA-C	6.01	117.91	111.36
1	A	207	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	337	MET	O-C-N	-6.00	114.02	122.06
1	A	119	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	B	296	ASN	CA-C-O	5.99	126.31	119.18
1	A	70	MET	CA-C-N	5.99	128.63	120.54
1	A	70	MET	C-N-CA	5.99	128.63	120.54
1	A	367	TRP	CA-C-O	-5.99	114.22	121.28
1	B	134	GLY	CA-C-O	5.98	127.14	122.29
1	B	12	ARG	O-C-N	5.98	129.79	123.03
1	B	179	GLU	CA-C-O	5.98	126.85	119.97
1	A	143	GLN	O-C-N	-5.98	115.78	122.12
1	B	100	VAL	CA-C-O	-5.98	113.83	120.46
1	A	124	ILE	O-C-N	5.97	129.52	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLY	CA-C-N	5.97	128.77	120.29
1	A	211	GLY	C-N-CA	5.97	128.77	120.29
1	A	227	ASP	O-C-N	-5.97	114.45	121.32
1	A	345	ILE	N-CA-CB	5.97	117.54	110.55
1	B	55	LYS	CA-C-O	-5.97	114.55	120.82
1	A	360	THR	CA-C-O	-5.97	114.66	121.58
1	A	371	PHE	CA-C-O	-5.97	113.87	120.38
1	B	276	SER	O-C-N	-5.97	115.79	122.12
1	A	270	ASP	O-C-N	-5.96	115.35	122.63
1	B	296	ASN	O-C-N	-5.95	113.96	122.41
1	B	186	VAL	CA-CB-CG1	5.94	120.50	110.40
1	A	276	SER	CA-CB-OG	5.94	122.97	111.10
1	A	381	THR	OG1-CB-CG2	-5.93	97.44	109.30
1	B	79	GLU	O-C-N	-5.93	113.78	122.43
1	B	77	LEU	CA-C-N	5.92	128.22	120.28
1	B	77	LEU	C-N-CA	5.92	128.22	120.28
1	B	244	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	300	TRP	N-CA-C	5.92	119.05	109.40
1	B	86	TYR	O-C-N	-5.89	115.43	122.15
1	B	80	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	317	LEU	CA-C-N	5.88	131.33	122.68
1	A	317	LEU	C-N-CA	5.88	131.33	122.68
1	A	293	SER	CA-C-O	5.87	125.24	118.55
1	B	38	ASP	CA-C-O	-5.86	114.67	120.82
1	A	56	PHE	O-C-N	-5.86	116.04	122.07
1	A	234	LYS	N-CA-CB	-5.85	101.44	111.39
1	B	184	ALA	O-C-N	5.85	130.03	122.89
1	B	328	ARG	CD-NE-CZ	5.85	132.58	124.40
1	A	294	ASP	CB-CG-OD1	5.84	131.83	118.40
1	B	11	GLN	CA-C-O	-5.84	112.07	119.31
1	B	75	GLU	N-CA-C	-5.84	104.92	111.28
1	A	33	GLN	CA-C-O	5.84	126.61	120.42
1	B	201	PRO	O-C-N	-5.84	115.78	123.13
1	B	133	SER	CA-C-O	5.83	127.92	120.57
1	B	106	GLY	CA-C-O	-5.83	114.74	120.75
1	B	370	LEU	O-C-N	-5.83	115.66	123.23
1	A	371	PHE	N-CA-C	5.83	118.45	109.07
1	B	316	LYS	N-CA-C	5.83	117.63	111.28
1	B	144	LEU	CA-C-O	5.82	126.67	119.97
1	B	288	GLU	CA-C-O	5.81	123.98	118.34
1	B	375	PRO	O-C-N	-5.81	115.76	122.85
1	B	56	PHE	O-C-N	5.81	128.28	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CA-C-O	-5.80	114.27	120.42
1	B	260	GLU	N-CA-CB	-5.80	101.29	110.22
1	B	75	GLU	N-CA-CB	5.79	118.63	110.12
1	A	132	THR	CA-CB-CG2	5.78	120.32	110.50
1	B	313	VAL	CA-C-O	-5.77	114.73	120.85
1	B	141	ASP	CA-C-O	5.77	126.53	120.42
1	B	329	GLU	O-C-N	-5.76	116.02	122.12
1	B	81	PRO	CA-C-O	5.75	128.30	119.55
1	B	95	GLN	CB-CA-C	-5.75	101.24	110.79
1	B	139	GLY	O-C-N	5.75	129.95	122.71
1	B	290	LEU	CA-C-O	5.75	126.08	119.35
1	A	242	THR	CA-C-O	-5.75	114.91	121.40
1	B	210	VAL	CA-C-O	5.74	127.26	121.17
1	B	5	SER	CA-C-O	-5.74	113.37	119.97
1	B	42	LYS	N-CA-CB	5.74	118.30	109.98
1	A	389	ILE	CB-CA-C	5.74	123.07	111.60
1	B	67	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	124	ILE	CA-C-O	-5.73	113.98	120.74
1	B	293	SER	CA-C-O	-5.72	112.03	118.55
1	B	177	LEU	CA-C-O	-5.72	114.78	120.90
1	A	182	LYS	O-C-N	-5.71	116.20	123.06
1	A	208	SER	O-C-N	-5.71	115.54	122.22
1	B	129	VAL	CA-C-O	-5.71	114.40	120.39
1	B	104	ARG	CD-NE-CZ	5.70	132.39	124.40
1	B	303	HIS	CA-C-O	-5.70	114.39	119.75
1	B	259	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	B	82	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	119	GLN	N-CA-CB	-5.69	103.14	109.74
1	B	311	ASP	CA-C-O	5.69	126.45	120.42
1	A	322	GLU	O-C-N	5.69	130.05	122.43
1	B	15	GLY	O-C-N	5.68	127.45	121.77
1	B	199	ARG	NH1-CZ-NH2	-5.68	111.92	119.30
1	A	362	GLY	CA-C-O	5.68	130.45	120.57
1	B	172	ARG	NH1-CZ-NH2	-5.67	111.93	119.30
1	B	257	HIS	O-C-N	5.67	130.05	123.30
1	A	102	VAL	CA-C-O	-5.65	112.38	119.95
1	A	292	ILE	CB-CG1-CD1	-5.65	101.94	113.80
1	B	227	ASP	CB-CA-C	-5.64	107.19	111.20
1	A	66	LYS	CB-CA-C	-5.63	99.47	110.11
1	B	259	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	B	356	ASN	OD1-CG-ND2	5.63	128.23	122.60
1	A	71	TYR	CA-C-O	-5.62	114.88	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	VAL	O-C-N	-5.62	115.44	121.80
1	B	35	THR	O-C-N	-5.62	114.61	122.37
1	A	43	ILE	CA-C-O	-5.62	113.23	120.03
1	A	129	VAL	O-C-N	5.62	129.33	123.26
1	B	42	LYS	N-CA-C	-5.61	104.80	111.03
1	A	372	GLY	CA-C-O	-5.61	115.14	120.64
1	B	296	ASN	CA-CB-CG	-5.61	106.99	112.60
1	B	38	ASP	N-CA-C	-5.60	105.08	111.07
1	A	255	ASP	CA-C-O	-5.59	114.84	121.16
1	A	255	ASP	CA-C-N	5.59	132.36	121.41
1	A	255	ASP	C-N-CA	5.59	132.36	121.41
1	B	52	LEU	CA-C-O	-5.58	113.21	119.79
1	B	30	CYS	O-C-N	-5.56	116.73	123.13
1	A	376	GLY	CA-C-O	-5.56	110.90	120.57
1	A	52	LEU	CA-C-O	5.55	126.65	120.82
1	B	325	ASN	CA-C-O	5.55	126.64	120.82
1	A	351	LYS	CA-C-N	5.54	128.16	120.29
1	A	351	LYS	C-N-CA	5.54	128.16	120.29
1	A	204	THR	CA-C-O	5.54	125.83	119.35
1	A	112	LYS	N-CA-CB	5.53	117.99	109.91
1	A	340	ALA	O-C-N	-5.53	115.47	122.27
1	A	328	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	B	107	LYS	CA-C-O	-5.52	114.70	120.55
1	B	380	GLU	OE1-CD-OE2	-5.52	109.65	122.90
1	A	233	GLU	OE1-CD-OE2	5.52	136.14	122.90
1	B	190	CYS	CA-C-O	-5.52	114.42	120.43
1	B	282	ALA	CA-C-O	-5.51	115.03	120.82
1	B	212	GLN	CG-CD-OE1	5.51	131.82	120.80
1	B	60	CYS	CA-C-O	-5.51	114.58	120.42
1	A	177	LEU	O-C-N	-5.50	116.29	122.12
1	B	261	ALA	N-CA-CB	-5.50	102.54	110.56
1	B	170	VAL	O-C-N	5.49	128.01	121.80
1	A	8	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	B	197	THR	CA-C-N	5.47	128.87	121.05
1	B	197	THR	C-N-CA	5.47	128.87	121.05
1	A	118	GLY	CA-C-O	-5.46	112.95	119.07
1	A	104	ARG	CA-C-O	5.46	126.75	120.90
1	B	185	ARG	N-CA-C	-5.45	99.40	108.34
1	B	137	MET	CG-SD-CE	-5.45	88.92	100.90
1	A	142	TYR	CA-C-N	-5.44	112.99	120.28
1	A	142	TYR	C-N-CA	-5.44	112.99	120.28
1	B	343	LEU	O-C-N	5.44	128.35	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	LEU	CA-C-O	-5.43	114.76	120.58
1	B	62	LYS	CA-CB-CG	5.43	124.96	114.10
1	B	317	LEU	N-CA-C	5.43	119.91	113.28
1	A	363	GLU	O-C-N	-5.43	112.82	122.21
1	A	49	LYS	CA-C-O	5.42	129.42	122.64
1	A	56	PHE	CB-CA-C	-5.42	102.36	110.88
1	A	254	ILE	CA-C-O	-5.42	114.99	120.31
1	A	362	GLY	O-C-N	-5.42	115.65	122.70
1	B	51	GLU	CA-C-O	5.42	126.05	119.38
1	B	146	LYS	CA-CB-CG	5.42	124.93	114.10
1	A	92	ASP	N-CA-CB	5.42	118.17	110.16
1	A	240	VAL	CB-CA-C	-5.42	105.60	110.91
1	B	37	PRO	CA-C-O	-5.41	111.50	120.05
1	A	388	ALA	CA-C-N	5.41	131.44	121.70
1	A	388	ALA	C-N-CA	5.41	131.44	121.70
1	B	385	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
1	A	238	GLU	CA-C-O	-5.41	115.05	121.16
1	A	285	GLU	O-C-N	-5.40	116.39	122.12
1	A	7	ILE	N-CA-C	-5.39	105.25	110.42
1	A	110	ALA	CA-C-O	5.39	126.26	120.55
1	B	80	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	184	ALA	CA-C-O	-5.38	115.14	121.16
1	B	284	VAL	N-CA-CB	5.37	120.49	110.77
1	B	206	LEU	O-C-N	-5.36	115.67	122.27
1	B	52	LEU	N-CA-C	-5.35	105.49	112.23
1	A	104	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	328	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	B	156	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	B	261	ALA	CA-C-O	5.34	125.81	119.56
1	A	59	MET	O-C-N	-5.34	116.57	122.07
1	A	169	THR	CA-C-O	5.34	126.61	120.90
1	B	257	HIS	CA-C-O	-5.33	114.60	120.36
1	A	89	PRO	CA-C-O	5.33	126.87	121.27
1	A	312	GLN	CB-CA-C	5.33	120.90	110.67
1	B	19	ILE	CA-C-O	-5.31	114.47	120.74
1	A	317	LEU	N-CA-C	5.31	119.76	113.28
1	A	96	ASP	N-CA-C	-5.30	105.50	111.28
1	A	207	ASP	CA-C-O	-5.30	115.23	120.90
1	A	8	ARG	NH1-CZ-NH2	-5.30	112.41	119.30
1	A	369	VAL	O-C-N	-5.29	117.17	123.05
1	B	15	GLY	CA-C-O	-5.29	113.95	121.52
1	B	12	ARG	CD-NE-CZ	5.29	131.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CA-C-O	-5.29	115.62	121.28
1	A	285	GLU	CB-CG-CD	5.28	121.58	112.60
1	A	263	LEU	CA-C-O	-5.27	114.94	120.58
1	A	17	ALA	CA-C-O	5.27	126.99	121.19
1	A	342	VAL	CB-CA-C	5.27	120.80	112.26
1	B	298	ILE	CB-CA-C	-5.27	103.32	110.90
1	B	143	GLN	CG-CD-OE1	5.26	131.32	120.80
1	A	333	GLU	N-CA-C	5.26	119.41	112.89
1	B	312	GLN	CG-CD-OE1	5.26	131.32	120.80
1	B	26	ASN	N-CA-C	-5.26	102.15	108.25
1	B	169	THR	CB-CA-C	-5.25	102.07	110.79
1	A	140	ALA	N-CA-CB	5.25	118.42	110.28
1	A	331	LEU	CB-CA-C	-5.25	102.07	110.79
1	A	230	PRO	O-C-N	-5.25	116.45	122.85
1	B	345	ILE	CA-C-O	5.25	126.73	121.17
1	B	377	LEU	O-C-N	-5.24	115.62	122.59
1	B	74	GLU	N-CA-C	-5.24	105.57	111.28
1	A	344	PHE	N-CA-CB	5.23	117.81	110.12
1	B	205	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	B	308	ALA	O-C-N	-5.21	115.86	122.27
1	B	54	GLU	CA-C-O	5.21	126.29	120.82
1	A	348	GLU	OE1-CD-OE2	-5.20	110.41	122.90
1	A	50	THR	CA-C-N	5.20	127.19	120.44
1	A	50	THR	C-N-CA	5.20	127.19	120.44
1	A	26	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	45	ASN	CB-CA-C	-5.19	104.36	111.73
1	B	238	GLU	N-CA-CB	5.19	119.04	110.69
1	A	343	LEU	CA-C-N	5.18	127.23	120.28
1	A	343	LEU	C-N-CA	5.18	127.23	120.28
1	A	305	GLY	CA-C-O	5.18	125.88	120.80
1	A	31	VAL	O-C-N	-5.17	116.14	122.97
1	A	292	ILE	N-CA-C	5.17	115.41	108.17
1	B	93	ALA	N-CA-CB	-5.17	102.51	110.12
1	B	288	GLU	O-C-N	-5.17	115.85	120.71
1	A	147	LEU	N-CA-CB	5.17	117.72	110.12
1	B	110	ALA	CA-C-O	-5.17	114.25	120.10
1	B	386	SER	N-CA-CB	-5.17	103.00	110.45
1	A	278	ASN	CA-CB-CG	-5.17	107.43	112.60
1	A	110	ALA	O-C-N	-5.17	116.64	122.12
1	A	35	THR	CA-C-O	-5.16	113.52	119.56
1	B	98	VAL	N-CA-C	5.16	118.36	111.44
1	A	322	GLU	CB-CA-C	-5.16	99.52	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ASP	N-CA-CB	5.16	117.49	110.01
1	B	125	THR	CA-C-N	5.16	130.80	122.29
1	B	125	THR	C-N-CA	5.16	130.80	122.29
1	A	82	ASN	CA-C-O	5.15	125.90	119.97
1	B	135	VAL	CA-CB-CG1	5.15	119.16	110.40
1	B	104	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	B	289	PRO	CA-C-O	-5.15	111.11	118.89
1	B	215	PHE	N-CA-C	5.15	118.33	110.20
1	A	251	GLU	O-C-N	-5.15	116.57	122.95
1	A	350	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	B	172	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	383	VAL	CA-C-O	5.14	126.07	120.57
1	B	373	PHE	CA-C-N	-5.13	113.81	121.87
1	B	373	PHE	C-N-CA	-5.13	113.81	121.87
1	B	384	LEU	CA-C-N	-5.13	114.75	122.81
1	B	384	LEU	C-N-CA	-5.13	114.75	122.81
1	A	275	VAL	CB-CA-C	-5.13	105.41	111.97
1	A	35	THR	O-C-N	5.13	128.49	122.34
1	A	146	LYS	N-CA-C	-5.13	105.60	111.14
1	B	204	THR	O-C-N	-5.12	115.78	122.39
1	A	203	ASP	CA-C-O	-5.12	112.39	119.05
1	A	289	PRO	O-C-N	-5.12	115.34	122.30
1	A	301	ILE	N-CA-C	-5.12	100.16	107.78
1	A	16	PRO	CB-CA-C	-5.12	104.86	111.46
1	B	124	ILE	CB-CA-C	5.11	116.75	111.23
1	A	95	GLN	CA-C-O	5.11	126.19	120.82
1	B	336	ASN	CB-CG-ND2	5.11	124.06	116.40
1	B	358	LEU	O-C-N	-5.11	116.42	122.65
1	B	22	ILE	O-C-N	5.10	129.01	123.09
1	B	59	MET	O-C-N	5.09	127.31	122.07
1	A	153	TYR	CA-C-O	5.08	125.83	119.78
1	A	364	GLY	CA-C-O	-5.08	113.38	119.06
1	B	85	GLU	CA-C-O	5.06	127.78	121.81
1	B	351	LYS	CA-C-O	-5.06	115.19	120.55
1	B	339	SER	N-CA-C	5.05	118.22	111.75
1	A	101	GLU	OE1-CD-OE2	-5.05	110.78	122.90
1	A	171	LEU	N-CA-C	5.04	116.86	111.36
1	A	201	PRO	N-CA-C	5.04	120.10	111.68
1	A	79	GLU	CA-CB-CG	-5.04	104.02	114.10
1	B	38	ASP	O-C-N	5.04	127.26	122.07
1	B	57	GLN	N-CA-CB	5.04	117.48	109.82
1	B	196	VAL	CG1-CB-CG2	-5.04	99.71	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	GLY	O-C-N	5.04	128.07	122.68
1	B	119	GLN	CG-CD-OE1	-5.04	110.72	120.80
1	A	91	LEU	CA-C-O	-5.04	114.41	120.10
1	B	340	ALA	N-CA-CB	-5.04	102.03	110.39
1	B	274	ILE	CA-C-O	-5.03	115.52	120.85
1	B	371	PHE	CB-CG-CD2	5.03	129.25	120.70
1	B	298	ILE	CA-C-N	-5.03	113.47	122.07
1	B	298	ILE	C-N-CA	-5.03	113.47	122.07
1	A	320	LYS	CA-C-N	5.02	125.29	119.47
1	A	320	LYS	C-N-CA	5.02	125.29	119.47
1	A	235	PRO	CA-C-O	-5.02	115.69	121.36
1	B	171	LEU	CA-C-N	5.01	127.31	120.54
1	B	171	LEU	C-N-CA	5.01	127.31	120.54
1	B	311	ASP	CA-CB-CG	-5.01	107.58	112.60
1	B	186	VAL	N-CA-C	5.00	115.52	108.36
1	A	29	ASN	O-C-N	-5.00	116.02	122.77
1	B	80	ASN	CA-C-N	5.00	124.78	119.28
1	B	80	ASN	C-N-CA	5.00	124.78	119.28
1	B	99	VAL	O-C-N	5.00	127.76	122.06
1	A	198	PHE	O-C-N	5.00	129.06	123.06
1	B	269	LYS	CA-C-N	-5.00	115.36	122.41
1	B	269	LYS	C-N-CA	-5.00	115.36	122.41

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	THR	Mainchain
1	A	137	MET	Mainchain,Peptide
1	A	166	ALA	Mainchain
1	A	248	PRO	Mainchain
1	A	337	MET	Mainchain
1	A	376	GLY	Mainchain,Peptide
1	A	56	PHE	Mainchain
1	B	118	GLY	Mainchain
1	B	137	MET	Mainchain,Peptide
1	B	166	ALA	Mainchain
1	B	181	ASN	Mainchain
1	B	187	LEU	Mainchain
1	B	213	ALA	Mainchain
1	B	265	PHE	Mainchain
1	B	376	GLY	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	2995	0	3043	50	1
1	B	2995	0	3043	63	1
2	A	103	0	61	13	0
2	B	103	0	61	10	0
3	A	232	0	0	4	7
3	B	208	0	0	8	6
All	All	6636	0	6208	119	8

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

All (119) 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:B:51:GLU:HA	3:B:545:HOH:O	1.62	0.99
1:B:59:MET:HE2	2:B:391[B]:HXC:H1'	1.44	0.98
1:A:59:MET:HE2	2:A:390[B]:HXC:H1'	1.52	0.92
1:A:309:ILE:HD11	2:A:390[B]:HXC:HP12	1.57	0.85
1:A:197:THR:HG22	1:A:263:LEU:HD23	1.60	0.83
1:B:78:LYS:HE3	1:B:79:GLU:CG	2.13	0.77
1:B:78:LYS:HE3	1:B:79:GLU:HG2	1.66	0.76
1:A:75:GLU:O	1:A:78:LYS:HD3	1.87	0.75
1:A:288:GLU:HG2	3:A:619:HOH:O	1.87	0.72
1:B:98:VAL:HG11	1:B:196:VAL:HG23	1.72	0.71
1:A:197:THR:CG2	1:A:263:LEU:HD23	2.26	0.64
2:A:390[A]:HXC:P3	2:A:390[A]:HXC:O2'	2.57	0.63
1:A:59:MET:HG2	2:A:390[B]:HXC:H4'	1.81	0.62
1:B:309:ILE:HD11	2:B:391[B]:HXC:HP12	1.83	0.61
1:A:240:VAL:HG21	1:A:367:TRP:HZ3	1.66	0.61
1:B:271:VAL:HG11	2:B:391[B]:HXC:HP11	1.84	0.59
1:A:78:LYS:HB2	3:A:621:HOH:O	2.02	0.59
1:A:42:LYS:HG3	1:A:47:GLU:OE2	2.02	0.59
2:B:391[A]:HXC:HP83	2:B:391[A]:HXC:H8	1.84	0.59
2:A:390[A]:HXC:HP11	2:A:390[A]:HXC:OP1	2.03	0.58
1:B:54:GLU:HB2	3:B:545:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ALA:O	1:B:97:MET:HG3	2.03	0.58
1:A:271:VAL:HG11	2:A:390[B]:HXC:HP11	1.88	0.55
1:B:164:SER:HB3	1:B:303:HIS:CE1	2.43	0.54
1:A:47:GLU:HG3	3:A:609:HOH:O	2.07	0.54
1:B:129:VAL:HG21	1:B:141:ASP:HA	1.88	0.54
1:A:95:GLN:OE1	1:A:134:GLY:HA2	2.07	0.54
1:B:55:LYS:HD3	2:B:391[B]:HXC:O33	2.08	0.54
1:B:104:ARG:NH1	1:B:108:GLU:OE2	2.41	0.53
1:A:240:VAL:HG21	1:A:367:TRP:CZ3	2.43	0.53
1:A:104:ARG:NH1	1:A:108:GLU:OE2	2.42	0.52
1:A:377:LEU:C	1:A:377:LEU:HD23	2.35	0.52
1:A:29:ASN:HB3	1:A:70:MET:O	2.09	0.52
1:B:42:LYS:HG3	1:B:47:GLU:OE2	2.10	0.52
1:A:107:LYS:HD2	1:A:147:LEU:HB3	1.91	0.52
1:B:315:GLN:HG3	3:B:493:HOH:O	2.10	0.51
1:B:87:MET:HE1	1:B:264:THR:HG21	1.92	0.51
1:A:3:SER:OG	1:A:6:GLU:HG3	2.11	0.50
1:B:292:ILE:HD12	1:B:293:SER:N	2.27	0.50
1:B:57:GLN:NE2	3:B:395:HOH:O	2.42	0.50
1:B:75:GLU:O	1:B:79:GLU:HG3	2.12	0.50
1:B:377:LEU:HD23	1:B:377:LEU:C	2.37	0.50
1:A:29:ASN:O	1:A:69:TYR:HA	2.12	0.50
2:A:390[A]:HXC:OP1	2:A:390[A]:HXC:CP1	2.56	0.50
1:A:164:SER:HB3	1:A:303:HIS:CE1	2.47	0.49
1:A:1:MET:SD	1:A:2:VAL:HG23	2.52	0.49
1:B:36:TYR:HB3	1:B:37:PRO:HD3	1.93	0.49
1:A:210:VAL:HG21	2:A:390[B]:HXC:C5	2.43	0.49
1:B:188:VAL:O	1:B:221:ALA:HA	2.12	0.49
1:A:162:GLN:HB3	1:A:166:ALA:HB2	1.93	0.49
2:B:391[B]:HXC:H5'2	2:B:391[B]:HXC:HPB2	1.93	0.49
1:B:159:MET:HB3	1:B:162:GLN:CD	2.38	0.48
1:B:158:MET:HE3	1:B:159:MET:N	2.29	0.47
1:A:36:TYR:N	1:A:37:PRO:CD	2.78	0.47
1:A:271:VAL:HB	1:A:272:PRO:HD3	1.95	0.47
1:B:135:VAL:HA	1:B:160:TYR:CE1	2.50	0.47
1:A:241:TRP:CH2	1:A:285:GLU:HG2	2.51	0.46
1:B:72:LEU:HD11	1:B:195:ALA:HA	1.97	0.46
1:B:42:LYS:HG3	1:B:47:GLU:CD	2.41	0.46
1:B:49:LYS:HB2	3:B:463:HOH:O	2.15	0.46
1:A:59:MET:HE2	2:A:390[A]:HXC:H1'	1.97	0.46
1:B:90:SER:O	1:B:94:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLU:HG3	3:A:614:HOH:O	2.17	0.45
1:A:55:LYS:HE2	1:A:55:LYS:HB2	1.72	0.44
1:A:55:LYS:HD3	2:A:390[B]:HXC:O33	2.17	0.44
1:A:230:PRO:O	1:A:231:GLU:HB2	2.17	0.44
1:B:52:LEU:HD22	1:B:203:ASP:HB3	1.98	0.44
1:B:302:ALA:O	1:B:303:HIS:C	2.59	0.44
1:B:54:GLU:HB3	1:B:58:ARG:HH12	1.82	0.44
1:A:87:MET:HE1	1:A:264:THR:HG21	1.99	0.44
1:B:29:ASN:HB3	1:B:70:MET:O	2.18	0.44
1:A:206:LEU:HB2	2:A:390[B]:HXC:H2	1.99	0.43
1:B:24:THR:HB	1:B:344:PHE:CZ	2.53	0.43
1:B:162:GLN:HB3	1:B:166:ALA:HB2	2.00	0.43
1:A:66:LYS:HD2	1:A:332:SER:OG	2.18	0.43
1:A:95:GLN:O	1:A:96:ASP:C	2.61	0.43
1:A:135:VAL:HA	1:A:160:TYR:CE1	2.54	0.43
1:B:389:ILE:N	1:B:389:ILE:HD13	2.34	0.43
1:B:54:GLU:CD	3:B:545:HOH:O	2.62	0.42
1:B:78:LYS:HE3	1:B:79:GLU:HG3	1.98	0.42
1:B:172:ARG:HA	1:B:242:THR:HG21	2.00	0.42
1:A:309:ILE:CD1	2:A:390[B]:HXC:HP12	2.37	0.42
1:B:42:LYS:HZ1	1:B:47:GLU:CD	2.28	0.42
1:B:62:LYS:HG2	2:B:391[A]:HXC:O6	2.18	0.42
1:B:132:THR:HG22	1:B:132:THR:O	2.20	0.42
1:B:210:VAL:HG21	2:B:391[B]:HXC:C5	2.49	0.42
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.90	0.42
1:B:36:TYR:N	1:B:37:PRO:CD	2.83	0.42
1:B:174:ALA:O	1:B:175:LYS:C	2.60	0.42
1:B:307:PRO:HG2	2:B:391[A]:HXC:HP92	2.01	0.42
1:B:46:SER:HB3	3:B:463:HOH:O	2.19	0.42
1:A:101:GLU:OE2	1:A:104:ARG:NH2	2.52	0.42
2:A:390[B]:HXC:HPB2	2:A:390[B]:HXC:H5'2	2.02	0.41
1:B:91:LEU:O	1:B:91:LEU:HG	2.20	0.41
1:B:151:ARG:HH11	1:B:151:ARG:HD2	1.54	0.41
1:B:309:ILE:CD1	2:B:391[B]:HXC:HP12	2.49	0.41
1:B:292:ILE:HD11	1:B:294:ASP:O	2.21	0.41
1:B:303:HIS:HD2	3:B:397:HOH:O	2.03	0.41
1:A:156:ARG:HH11	1:A:156:ARG:HD2	1.72	0.41
1:B:42:LYS:NZ	1:B:47:GLU:OE2	2.53	0.41
1:A:301:ILE:HG22	1:A:342:VAL:HG22	2.03	0.40
1:B:121:LYS:HD2	1:B:148:LEU:O	2.22	0.40
1:A:258:LEU:HA	1:A:258:LEU:HD12	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLY:O	1:B:268:LEU:HB2	2.21	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:550:HOH:O	3:B:392:HOH:O[3_554]	1.38	0.82
3:A:520:HOH:O	3:B:392:HOH:O[3_554]	1.58	0.62
3:A:516:HOH:O	3:B:469:HOH:O[3_554]	1.71	0.49
3:A:425:HOH:O	3:B:469:HOH:O[3_554]	1.77	0.43
3:A:545:HOH:O	3:B:469:HOH:O[3_554]	1.87	0.33
1:A:79:GLU:OE2	3:A:620:HOH:O[6_656]	2.14	0.06
3:A:616:HOH:O	3:B:559:HOH:O[6_656]	2.18	0.02
1:B:78:LYS:NZ	1:B:281:LYS:NZ[5_566]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	376 (97%)	9 (2%)	2 (0%)	24	16
1	B	387/389 (100%)	370 (96%)	16 (4%)	1 (0%)	36	29
All	All	774/778 (100%)	746 (96%)	25 (3%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	PRO
1	B	138	PRO
1	A	90	SER

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	325/325 (100%)	311 (96%)	14 (4%)	26	18
1	B	325/325 (100%)	307 (94%)	18 (6%)	19	11
All	All	650/650 (100%)	618 (95%)	32 (5%)	22	14

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	55	LYS
1	A	78	LYS
1	A	115	LYS
1	A	133	SER
1	A	235	PRO
1	A	268	LEU
1	A	269	LYS
1	A	279	ILE
1	A	284	VAL
1	A	292	ILE
1	A	342	VAL
1	A	355	GLN
1	A	389	ILE
1	B	1	MET
1	B	45	ASN
1	B	46	SER
1	B	50	THR
1	B	51	GLU
1	B	58	ARG
1	B	62	LYS
1	B	67	ARG
1	B	78	LYS
1	B	115	LYS
1	B	123	LYS
1	B	151	ARG
1	B	255	ASP

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Mol	Chain	Res	Type
1	B	284	VAL
1	B	292	ILE
1	B	341	CYS
1	B	342	VAL
1	B	350	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	181	ASN
1	A	303	HIS
1	A	312	GLN
1	A	315	GLN
1	B	26	ASN
1	B	45	ASN
1	B	205	HIS
1	B	303	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
2	HXC	B	391[A]	-	55,57,57	15.16	11 (20%)	77,83,83	6.71	20 (25%)
2	HXC	A	390[B]	-	55,57,57	1.88	11 (20%)	77,83,83	3.15	36 (46%)
2	HXC	B	391[B]	-	55,57,57	2.10	10 (18%)	77,83,83	3.57	38 (49%)
2	HXC	A	390[A]	-	55,57,57	13.71	10 (18%)	77,83,83	6.01	26 (33%)

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
2	HXC	B	391[A]	-	-	21/56/72/72	0/3/3/3
2	HXC	A	390[B]	-	-	20/56/72/72	0/3/3/3
2	HXC	B	391[B]	-	-	20/56/72/72	0/3/3/3
2	HXC	A	390[A]	-	-	15/56/72/72	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391[A]	HXC	CM1-S	111.75	4.39	1.76
2	A	390[A]	HXC	CM1-S	100.96	4.14	1.76
2	B	391[A]	HXC	CM3-CM2	-7.45	1.24	1.52
2	B	391[B]	HXC	CM3-CM2	-7.45	1.24	1.52
2	A	390[A]	HXC	CM3-CM2	-7.04	1.26	1.52
2	A	390[B]	HXC	CM3-CM2	-7.04	1.26	1.52
2	B	391[B]	HXC	CPB-CPA	5.39	1.61	1.52
2	A	390[B]	HXC	CP2-NP1	4.97	1.57	1.46
2	A	390[B]	HXC	CPB-CPA	4.90	1.60	1.52
2	B	391[B]	HXC	CP2-NP1	4.71	1.56	1.46
2	B	391[B]	HXC	C2-N3	-4.57	1.25	1.33
2	B	391[B]	HXC	CM1-S	4.32	1.86	1.76
2	B	391[B]	HXC	CP5-NP2	4.11	1.55	1.46
2	A	390[A]	HXC	CP2-NP1	3.99	1.55	1.46
2	B	391[B]	HXC	P3-O33	3.86	1.62	1.50
2	B	391[A]	HXC	CM2-CM1	3.84	1.54	1.50
2	B	391[B]	HXC	CM2-CM1	3.84	1.54	1.50
2	A	390[B]	HXC	P3-O33	3.54	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	390[B]	HXC	CM1-S	3.40	1.84	1.76
2	B	391[A]	HXC	CP5-NP2	3.28	1.53	1.46
2	B	391[A]	HXC	P2-O7	-3.14	1.47	1.59
2	B	391[A]	HXC	P3-O33	3.10	1.60	1.50
2	B	391[B]	HXC	P2-O7	-2.93	1.47	1.59
2	A	390[A]	HXC	P3-O33	2.92	1.59	1.50
2	A	390[A]	HXC	P2-O7	-2.88	1.48	1.59
2	A	390[B]	HXC	C2-N3	-2.85	1.28	1.33
2	A	390[A]	HXC	CM2-CM1	2.67	1.53	1.50
2	A	390[B]	HXC	CM2-CM1	2.67	1.53	1.50
2	A	390[B]	HXC	P2-O7	-2.67	1.48	1.59
2	A	390[A]	HXC	CP5-NP2	2.64	1.52	1.46
2	A	390[B]	HXC	CP5-NP2	2.59	1.52	1.46
2	B	391[A]	HXC	CP2-NP1	2.44	1.51	1.46
2	A	390[A]	HXC	CPB-CPA	2.42	1.56	1.52
2	A	390[A]	HXC	C2-N1	2.37	1.38	1.33
2	A	390[B]	HXC	CP1-S	2.26	1.91	1.81
2	A	390[A]	HXC	OM2-CM1	2.22	1.24	1.21
2	A	390[B]	HXC	OM2-CM1	2.22	1.24	1.21
2	B	391[A]	HXC	CPB-CPA	2.15	1.56	1.52
2	B	391[A]	HXC	C2-N3	-2.13	1.30	1.33
2	B	391[A]	HXC	P3-O32	-2.09	1.47	1.54
2	B	391[A]	HXC	C2-N1	2.06	1.37	1.33
2	B	391[B]	HXC	OP3-CP7	2.05	1.45	1.42

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391[A]	HXC	OM2-CM1-S	-31.29	82.88	122.68
2	B	391[A]	HXC	O4'-C4'-C3'	-27.07	47.80	104.92
2	A	390[A]	HXC	O32-P3-O33	-26.61	7.16	110.83
2	A	390[A]	HXC	OM2-CM1-S	-26.59	88.85	122.68
2	B	391[A]	HXC	CP1-S-CM1	-25.54	26.34	101.84
2	B	391[A]	HXC	CM2-CM1-S	-22.80	86.22	113.40
2	A	390[A]	HXC	CM2-CM1-S	-18.68	91.13	113.40
2	A	390[A]	HXC	CP1-S-CM1	-15.62	55.67	101.84
2	A	390[A]	HXC	C2'-C3'-C4'	-15.11	76.78	103.24
2	B	391[A]	HXC	C4'-O4'-C1'	-12.40	82.09	109.47
2	A	390[A]	HXC	C3'-C2'-C1'	10.83	123.72	99.89
2	B	391[A]	HXC	C3'-C2'-C1'	-10.43	76.94	99.89
2	B	391[B]	HXC	OP1-CP3-NP1	-9.30	104.78	123.03
2	B	391[B]	HXC	CP4-CP3-NP1	9.29	133.27	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390[A]	HXC	O4'-C1'-C2'	-8.57	88.27	106.62
2	A	390[B]	HXC	OP1-CP3-NP1	-8.53	106.28	123.03
2	B	391[B]	HXC	CM2-CM1-S	-8.49	103.28	113.40
2	A	390[B]	HXC	O2'-C2'-C1'	8.40	139.02	110.10
2	B	391[A]	HXC	O4'-C1'-C2'	-8.23	89.01	106.62
2	B	391[B]	HXC	OM2-CM1-S	8.07	132.95	122.68
2	B	391[A]	HXC	CM3-CM2-CM1	7.78	129.44	112.27
2	B	391[B]	HXC	CM3-CM2-CM1	7.78	129.44	112.27
2	B	391[B]	HXC	C2-N3-C4	-7.23	94.19	111.83
2	A	390[B]	HXC	C2-N3-C4	-7.07	94.56	111.83
2	A	390[A]	HXC	CP2-NP1-CP3	-6.99	109.80	122.82
2	A	390[B]	HXC	CP4-CP3-NP1	6.99	129.07	116.34
2	B	391[B]	HXC	O2'-C2'-C1'	6.88	133.81	110.10
2	B	391[B]	HXC	C5-C4-N9	-6.88	98.31	105.81
2	A	390[B]	HXC	CP5-NP2-CP6	-6.70	110.51	122.55
2	A	390[B]	HXC	CM2-CM1-S	-6.53	105.61	113.40
2	B	391[B]	HXC	O7-CPB-CPA	-6.44	100.19	110.55
2	A	390[B]	HXC	C4'-O4'-C1'	-6.38	95.38	109.47
2	B	391[B]	HXC	CP5-NP2-CP6	-6.18	111.45	122.55
2	A	390[A]	HXC	OP1-CP3-NP1	-5.81	111.64	123.03
2	B	391[B]	HXC	C4'-O4'-C1'	-5.79	96.69	109.47
2	A	390[A]	HXC	CP9-CPA-CP7	5.77	118.61	108.77
2	A	390[B]	HXC	C5-C6-N1	-5.67	103.12	117.51
2	A	390[A]	HXC	O3'-C3'-C4'	5.51	129.44	110.03
2	A	390[A]	HXC	CP4-CP3-NP1	5.28	125.96	116.34
2	A	390[B]	HXC	C6-C5-N7	-5.07	122.31	132.09
2	B	391[B]	HXC	CP5-CP4-CP3	5.03	120.77	112.39
2	B	391[A]	HXC	OP3-CP7-CP6	-4.92	88.86	109.38
2	A	390[A]	HXC	CM3-CM2-CM1	4.89	123.06	112.27
2	A	390[B]	HXC	CM3-CM2-CM1	4.89	123.06	112.27
2	A	390[B]	HXC	O4'-C4'-C3'	4.88	115.20	104.92
2	B	391[B]	HXC	C2'-C3'-C4'	-4.79	94.85	103.24
2	B	391[A]	HXC	CP2-NP1-CP3	-4.77	113.95	122.82
2	A	390[B]	HXC	O7-CPB-CPA	-4.75	102.91	110.55
2	A	390[B]	HXC	C2'-C3'-C4'	-4.71	94.98	103.24
2	B	391[B]	HXC	O4'-C4'-C3'	4.55	114.51	104.92
2	B	391[B]	HXC	C1'-N9-C8	-4.40	117.34	127.09
2	A	390[A]	HXC	OM2-CM1-CM2	4.16	128.77	123.98
2	A	390[B]	HXC	OM2-CM1-CM2	4.16	128.77	123.98
2	A	390[A]	HXC	CP5-NP2-CP6	-4.14	115.11	122.55
2	B	391[A]	HXC	O3'-C3'-C4'	4.13	124.58	110.03
2	B	391[B]	HXC	O4'-C1'-N9	3.98	115.73	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391[B]	HXC	N1-C2-N3	3.97	134.60	128.58
2	B	391[B]	HXC	C4-N9-C8	3.97	109.91	105.74
2	A	390[B]	HXC	CP9-CPA-CP7	3.92	115.44	108.77
2	A	390[B]	HXC	C5-C4-N9	-3.87	101.59	105.81
2	B	391[A]	HXC	CM5-CM4-CM3	3.81	148.66	115.25
2	B	391[B]	HXC	CM5-CM4-CM3	3.81	148.66	115.25
2	A	390[A]	HXC	C2'-C1'-N9	3.77	122.68	113.30
2	A	390[B]	HXC	C1'-N9-C8	-3.77	118.73	127.09
2	B	391[A]	HXC	CM4-CM3-CM2	3.72	126.79	113.13
2	B	391[B]	HXC	CM4-CM3-CM2	3.72	126.79	113.13
2	A	390[B]	HXC	C5-C6-N6	-3.58	114.43	123.29
2	B	391[B]	HXC	N9-C8-N7	-3.57	108.87	113.94
2	A	390[B]	HXC	O4'-C1'-N9	3.56	114.93	108.09
2	B	391[B]	HXC	N6-C6-N1	3.56	126.30	118.38
2	B	391[B]	HXC	CP9-CPA-CP7	3.54	114.80	108.77
2	B	391[A]	HXC	O12-P1-O6	3.50	116.72	107.27
2	A	390[B]	HXC	OP2-CP6-NP2	-3.38	115.83	122.98
2	B	391[B]	HXC	C4-C5-N7	3.32	114.38	110.58
2	B	391[A]	HXC	CP9-CPA-CPB	3.32	113.70	108.22
2	B	391[B]	HXC	C5-C6-N1	-3.30	109.12	117.51
2	A	390[B]	HXC	O3'-C3'-C4'	3.19	121.27	110.03
2	A	390[B]	HXC	CP2-NP1-CP3	-3.15	116.96	122.82
2	B	391[B]	HXC	O12-P1-O6	2.97	115.31	107.27
2	A	390[A]	HXC	C4-N9-C1'	2.94	133.51	126.63
2	B	391[B]	HXC	O3'-C3'-C4'	2.93	120.34	110.03
2	B	391[A]	HXC	CP9-CPA-CP7	-2.91	103.81	108.77
2	B	391[B]	HXC	C5-C4-N3	-2.86	122.77	126.72
2	A	390[B]	HXC	C3'-C2'-C1'	2.83	106.12	99.89
2	A	390[B]	HXC	CP1-CP2-NP1	2.78	118.23	112.41
2	A	390[A]	HXC	C5-C4-N3	-2.77	122.91	126.72
2	A	390[B]	HXC	CP4-CP5-NP2	2.76	117.88	112.00
2	A	390[A]	HXC	CM5-CM4-CM3	2.76	139.46	115.25
2	A	390[B]	HXC	CM5-CM4-CM3	2.76	139.46	115.25
2	B	391[B]	HXC	C3'-C2'-C1'	2.71	105.85	99.89
2	B	391[B]	HXC	C6-C5-N7	-2.65	126.98	132.09
2	A	390[A]	HXC	C1'-N9-C8	-2.64	121.24	127.09
2	A	390[A]	HXC	CP1-CP2-NP1	-2.58	107.02	112.41
2	A	390[B]	HXC	N1-C2-N3	2.56	132.46	128.58
2	B	391[B]	HXC	O32-P3-O33	-2.53	100.96	110.83
2	A	390[A]	HXC	O3'-P3-O33	-2.46	100.58	109.33
2	B	391[B]	HXC	OP2-CP6-NP2	-2.44	117.82	122.98
2	A	390[B]	HXC	CP9-CPA-CPB	-2.44	104.20	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390[B]	HXC	O32-P3-O33	-2.43	101.36	110.83
2	A	390[B]	HXC	O3'-C3'-C2'	2.43	120.38	111.68
2	B	391[A]	HXC	O3'-P3-O33	-2.42	100.69	109.33
2	A	390[B]	HXC	CP7-CP6-NP2	2.41	121.06	116.48
2	B	391[A]	HXC	O7-CPB-CPA	-2.37	106.73	110.55
2	B	391[A]	HXC	C2'-C1'-N9	2.34	119.13	113.30
2	A	390[B]	HXC	C4-N9-C8	2.34	108.20	105.74
2	A	390[A]	HXC	O2'-C2'-C3'	-2.34	104.65	111.19
2	B	391[B]	HXC	CP1-CP2-NP1	2.27	117.16	112.41
2	A	390[A]	HXC	OP3-CP7-CP6	2.24	118.73	109.38
2	B	391[A]	HXC	CP5-NP2-CP6	-2.24	118.53	122.55
2	A	390[B]	HXC	C4-N9-C1'	2.23	131.85	126.63
2	B	391[B]	HXC	O3'-C3'-C2'	2.21	119.60	111.68
2	A	390[B]	HXC	P1-O5'-C5'	2.20	133.94	121.35
2	B	391[B]	HXC	CP7-CP6-NP2	2.15	120.57	116.48
2	B	391[B]	HXC	C4-N9-C1'	2.15	131.67	126.63
2	A	390[A]	HXC	P3-O3'-C3'	-2.15	117.68	123.43
2	A	390[B]	HXC	C4-C5-N7	2.13	113.02	110.58
2	B	391[B]	HXC	CP2-NP1-CP3	-2.13	118.86	122.82
2	A	390[A]	HXC	OP2-CP6-NP2	2.10	127.43	122.98
2	A	390[B]	HXC	O31-P3-O3'	2.08	113.95	105.85
2	B	391[B]	HXC	OP3-CP7-CP6	-2.07	100.74	109.38

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	390[A]	HXC	C4'-C3'-O3'-P3
2	A	390[A]	HXC	C5'-O5'-P1-O12
2	A	390[A]	HXC	C5'-O5'-P1-O6
2	A	390[A]	HXC	CM2-CM1-S-CP1
2	A	390[A]	HXC	OM2-CM1-S-CP1
2	A	390[A]	HXC	CM1-CM2-CM3-CM4
2	A	390[B]	HXC	CPB-O7-P2-O21
2	A	390[B]	HXC	NP2-CP6-CP7-OP3
2	A	390[B]	HXC	OP2-CP6-NP2-CP5
2	A	390[B]	HXC	CP3-CP4-CP5-NP2
2	A	390[B]	HXC	CP2-CP1-S-CM1
2	A	390[B]	HXC	CM2-CM1-S-CP1
2	A	390[B]	HXC	OM2-CM1-S-CP1
2	A	390[B]	HXC	CM1-CM2-CM3-CM4
2	B	391[A]	HXC	C5'-O5'-P1-O11

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Mol	Chain	Res	Type	Atoms
2	B	391[A]	HXC	C5'-O5'-P1-O12
2	B	391[A]	HXC	C5'-O5'-P1-O6
2	B	391[A]	HXC	CP2-CP1-S-CM1
2	B	391[A]	HXC	CM2-CM1-S-CP1
2	B	391[A]	HXC	OM2-CM1-S-CP1
2	B	391[A]	HXC	CM1-CM2-CM3-CM4
2	B	391[B]	HXC	CPB-O7-P2-O6
2	B	391[B]	HXC	CP7-CPA-CPB-O7
2	B	391[B]	HXC	CP9-CPA-CPB-O7
2	B	391[B]	HXC	CP8-CPA-CPB-O7
2	B	391[B]	HXC	CP3-CP4-CP5-NP2
2	B	391[B]	HXC	CP2-CP1-S-CM1
2	B	391[B]	HXC	CM2-CM1-S-CP1
2	B	391[B]	HXC	OM2-CM1-S-CP1
2	B	391[B]	HXC	CM1-CM2-CM3-CM4
2	B	391[A]	HXC	O4'-C4'-C5'-O5'
2	B	391[A]	HXC	C4'-C3'-O3'-P3
2	A	390[B]	HXC	OP1-CP3-CP4-CP5
2	A	390[A]	HXC	C2'-C3'-O3'-P3
2	B	391[A]	HXC	C2'-C3'-O3'-P3
2	B	391[A]	HXC	S-CP1-CP2-NP1
2	B	391[A]	HXC	C2'-C1'-N9-C8
2	B	391[A]	HXC	CM2-CM3-CM4-CM5
2	B	391[B]	HXC	CM2-CM3-CM4-CM5
2	B	391[A]	HXC	C2'-C1'-N9-C4
2	B	391[A]	HXC	CM3-CM4-CM5-CM6
2	B	391[B]	HXC	CM3-CM4-CM5-CM6
2	B	391[B]	HXC	S-CP1-CP2-NP1
2	B	391[B]	HXC	OP2-CP6-NP2-CP5
2	A	390[B]	HXC	CP1-CP2-NP1-CP3
2	A	390[A]	HXC	S-CM1-CM2-CM3
2	B	391[A]	HXC	S-CM1-CM2-CM3
2	A	390[B]	HXC	C3'-O3'-P3-O33
2	A	390[A]	HXC	C5'-O5'-P1-O11
2	A	390[B]	HXC	C5'-O5'-P1-O12
2	A	390[B]	HXC	C5'-O5'-P1-O6
2	B	391[B]	HXC	CPB-O7-P2-O21
2	B	391[B]	HXC	OP1-CP3-CP4-CP5
2	A	390[A]	HXC	C2'-C1'-N9-C8
2	A	390[B]	HXC	OP1-CP3-NP1-CP2
2	A	390[A]	HXC	C2'-C1'-N9-C4
2	B	391[A]	HXC	C3'-O3'-P3-O31

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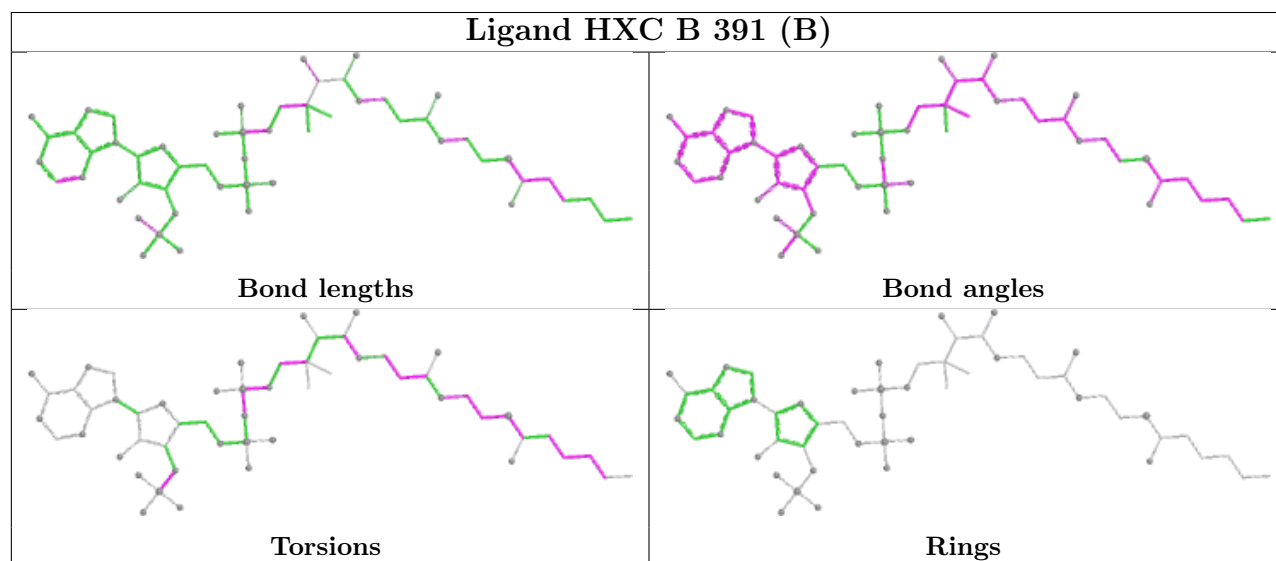
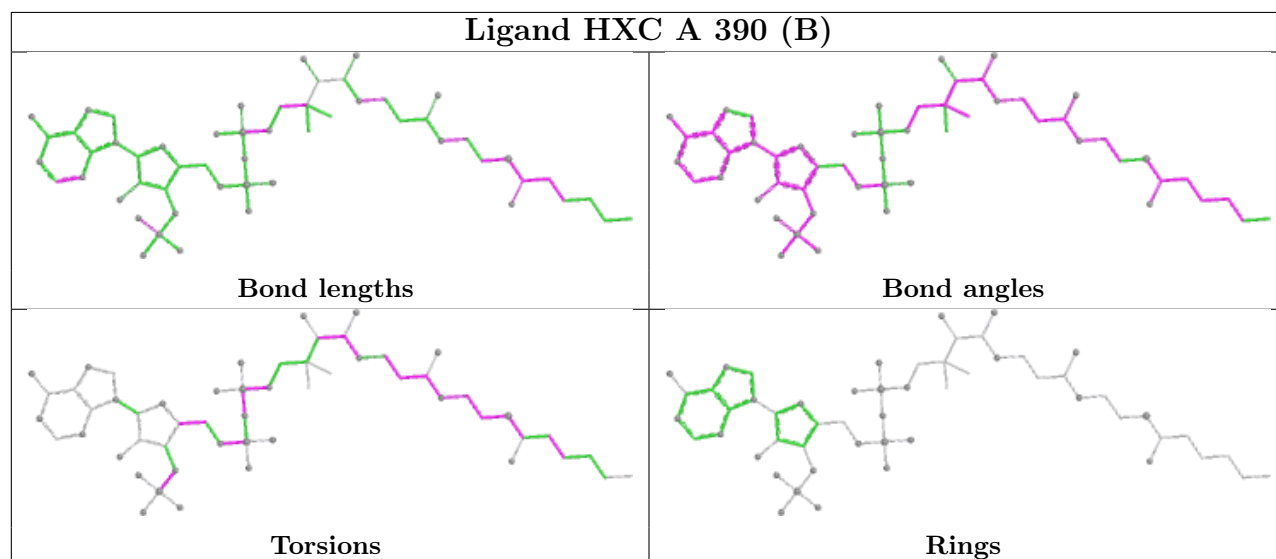
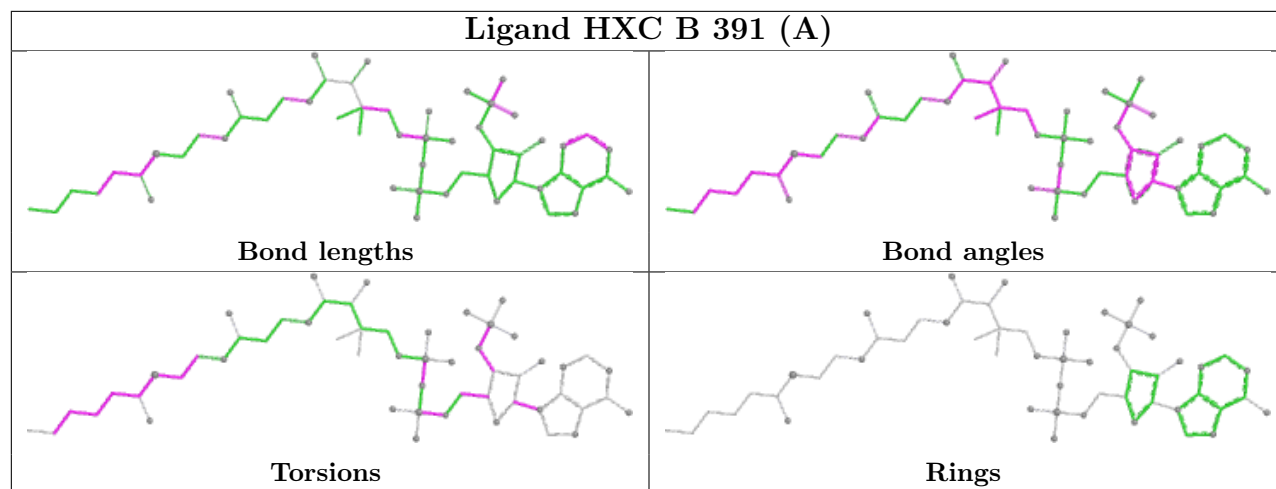
Mol	Chain	Res	Type	Atoms
2	B	391[B]	HXC	C3'-O3'-P3-O31
2	A	390[B]	HXC	S-CP1-CP2-NP1
2	A	390[A]	HXC	C3'-O3'-P3-O33
2	B	391[B]	HXC	C3'-O3'-P3-O33
2	A	390[B]	HXC	NP1-CP3-CP4-CP5
2	B	391[A]	HXC	O4'-C1'-N9-C8
2	B	391[B]	HXC	P1-O6-P2-O22
2	B	391[A]	HXC	C3'-C4'-C5'-O5'
2	A	390[A]	HXC	C3'-O3'-P3-O31
2	A	390[A]	HXC	NP1-CP3-CP4-CP5
2	B	391[B]	HXC	NP1-CP3-CP4-CP5
2	A	390[B]	HXC	NP2-CP6-CP7-CPA
2	B	391[A]	HXC	C3'-O3'-P3-O33
2	A	390[A]	HXC	OP1-CP3-CP4-CP5
2	A	390[B]	HXC	O4'-C4'-C5'-O5'
2	B	391[B]	HXC	CP1-CP2-NP1-CP3
2	A	390[B]	HXC	P1-O6-P2-O21
2	A	390[B]	HXC	P1-O6-P2-O22
2	B	391[A]	HXC	P1-O6-P2-O22

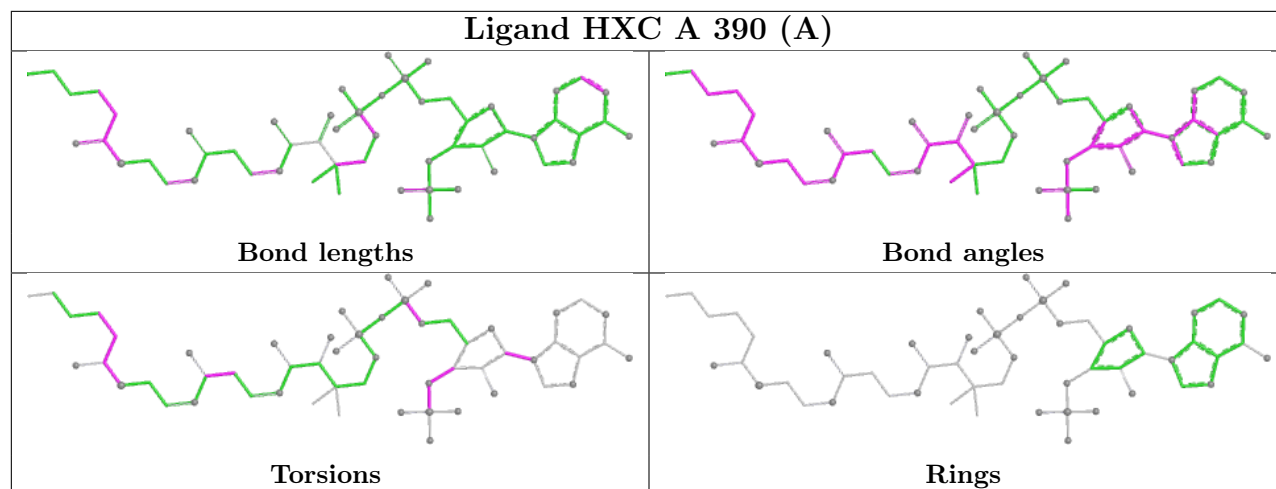
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	391[A]	HXC	3	0
2	A	390[B]	HXC	9	0
2	B	391[B]	HXC	7	0
2	A	390[A]	HXC	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	389/389 (100%)	0.02	9 (2%) 61 65	11, 20, 36, 63	0
1	B	389/389 (100%)	0.18	21 (5%) 31 33	11, 21, 43, 71	0
All	All	778/778 (100%)	0.10	30 (3%) 43 46	11, 20, 39, 71	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	THR	4.5
1	B	231	GLU	4.2
1	B	268	LEU	3.8
1	B	1	MET	3.8
1	A	1	MET	3.3
1	A	389	ILE	3.3
1	B	48	HIS	3.2
1	B	162	GLN	3.2
1	A	268	LEU	3.0
1	B	267	LEU	3.0
1	A	267	LEU	3.0
1	B	52	LEU	2.9
1	B	49	LYS	2.8
1	A	231	GLU	2.8
1	B	51	GLU	2.8
1	B	389	ILE	2.7
1	B	78	LYS	2.7
1	A	215	PHE	2.5
1	A	78	LYS	2.5
1	A	62	LYS	2.5
1	B	265	PHE	2.3
1	B	47	GLU	2.3
1	B	45	ASN	2.3
1	B	42	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	215	PHE	2.3
1	B	39	PHE	2.2
1	A	232	ILE	2.2
1	B	37	PRO	2.1
1	B	266	HIS	2.0
1	B	38	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

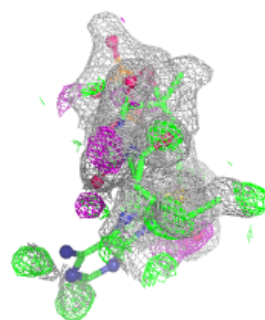
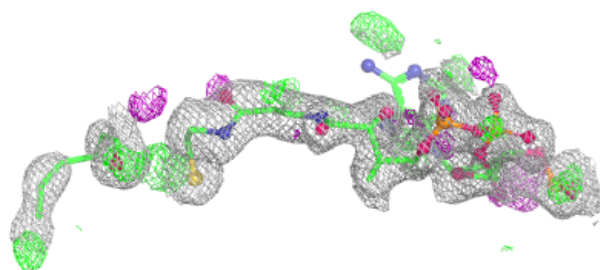
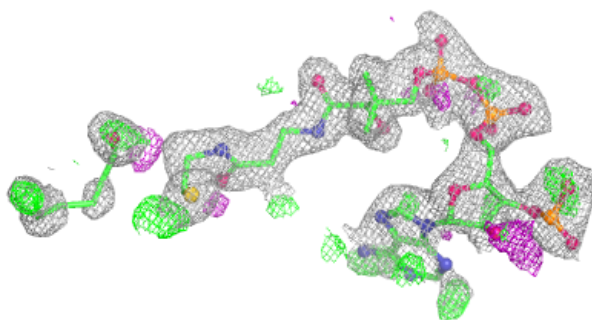
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HXC	A	390[A]	55/55	0.80	0.19	6,41,85,86	52
2	HXC	A	390[B]	55/55	0.80	0.19	6,58,75,76	52
2	HXC	B	391[A]	55/55	0.81	0.17	7,45,86,87	52
2	HXC	B	391[B]	55/55	0.81	0.17	7,55,75,75	52

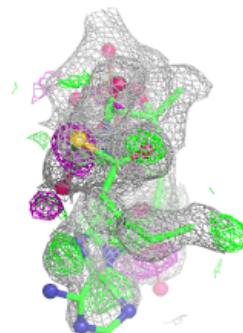
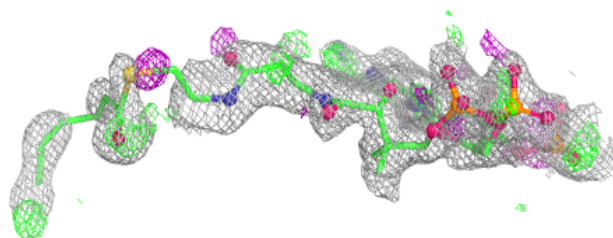
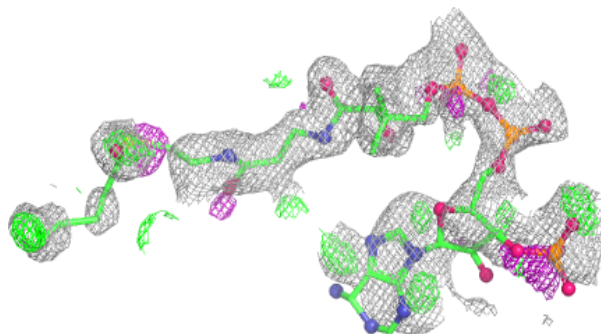
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HXC A 390 (A):

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

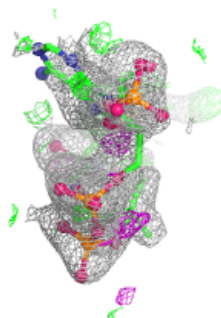
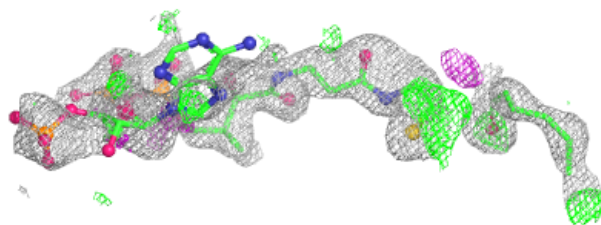
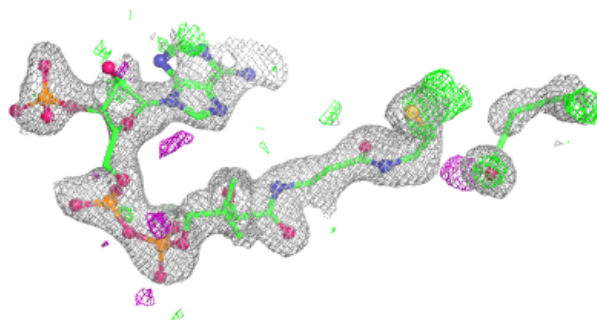
**Electron density around HXC A 390 (B):**

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

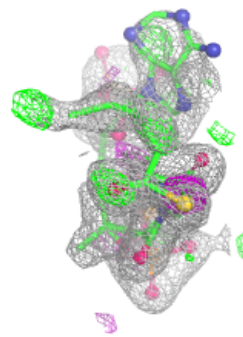
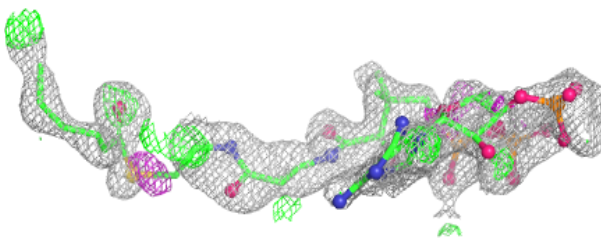
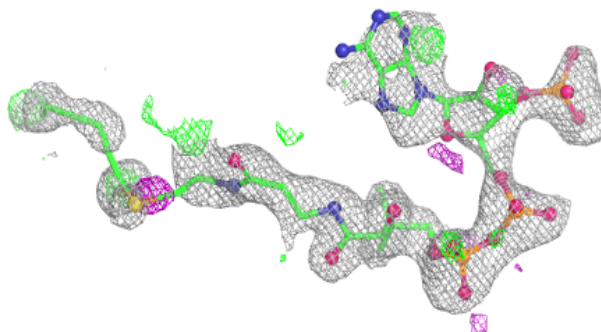


Electron density around HXC B 391 (A):

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

**Electron density around HXC B 391 (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.