



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:23 PM EDT

PDB ID : 1CHW  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

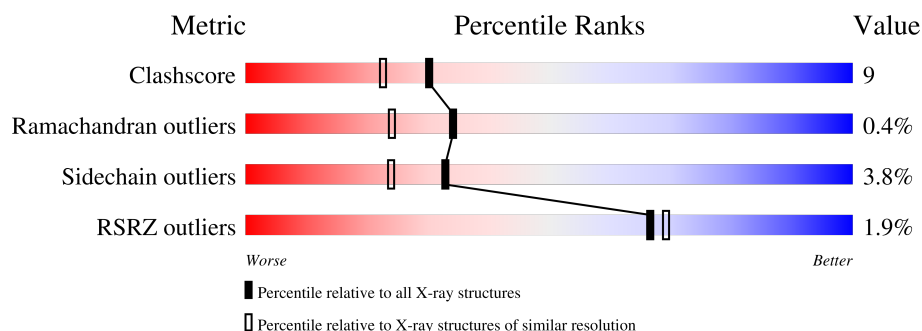
# 1 Overall quality at a glance

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	
1	B	389	

## 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.

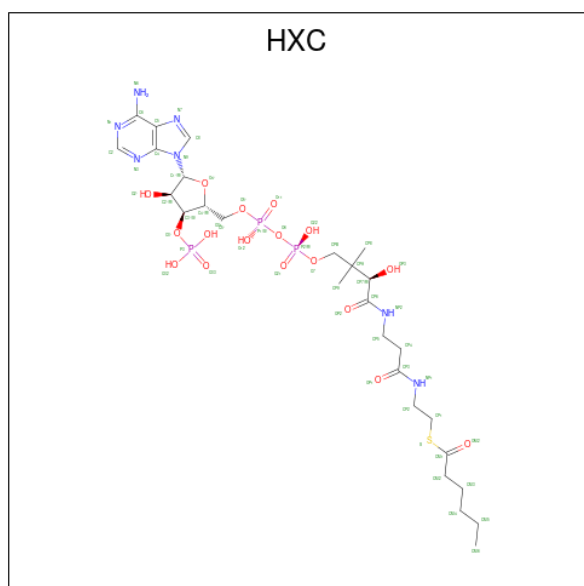
- Molecule 1 is a protein called PROTEIN (CHALCONE SYNTHASE).

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 (three-letter code: 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		

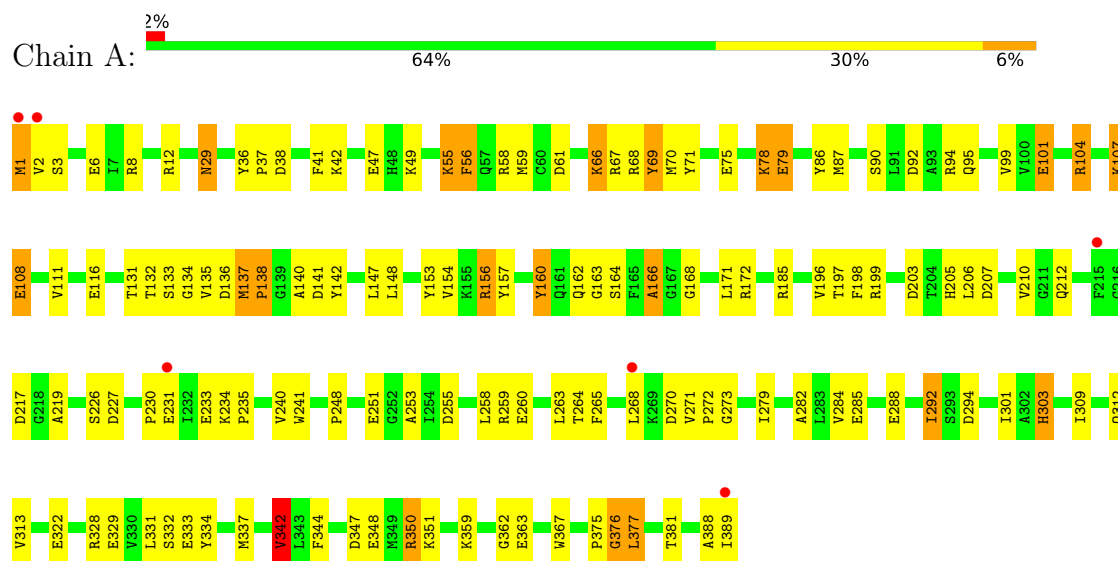
- Molecule 3 is water.

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

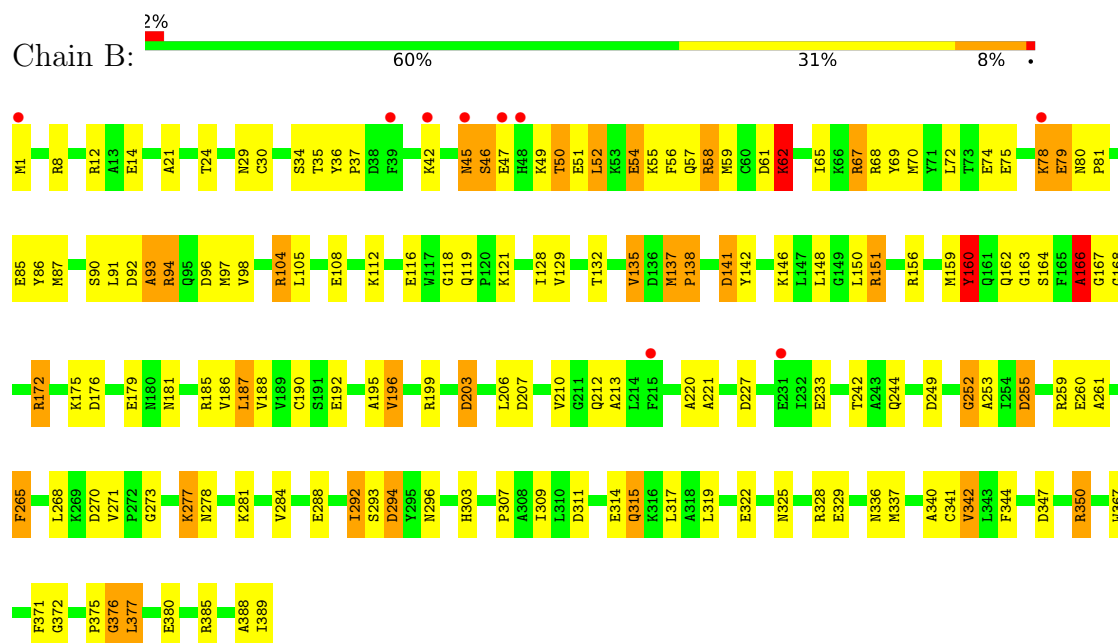
### 3 Residue-property plots [i](#)

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)



#### • 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, $\alpha$ , $\beta$ , $\gamma$	97.81Å 97.81Å 130.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.71 – 1.90 24.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.6 (70.71-1.90) 84.6 (24.03-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.89	0/3052	2.28	129/4130 (3.1%)
1	B	0.93	2/3052 (0.1%)	2.44	165/4130 (4.0%)
All	All	0.91	2/6104 (0.0%)	2.36	294/8260 (3.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	GLU	CD-OE1	6.18	1.32	1.25
1	B	50	THR	CB-OG1	5.88	1.55	1.43

All (294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH1	23.68	132.14	120.30
1	B	172	ARG	NE-CZ-NH2	22.31	131.45	120.30
1	A	12	ARG	NE-CZ-NH2	-22.22	109.19	120.30
1	B	67	ARG	NE-CZ-NH2	-19.07	110.76	120.30
1	B	68	ARG	NE-CZ-NH2	17.60	129.10	120.30
1	B	376	GLY	O-C-N	-16.31	96.61	122.70
1	B	8	ARG	NE-CZ-NH2	-16.13	112.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ARG	NE-CZ-NH2	15.89	128.25	120.30
1	A	185	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	B	104	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	A	294	ASP	CB-CG-OD1	15.03	131.83	118.30
1	B	67	ARG	NE-CZ-NH1	13.87	127.23	120.30
1	B	259	ARG	NE-CZ-NH1	13.79	127.20	120.30
1	B	68	ARG	NE-CZ-NH1	-13.73	113.43	120.30
1	A	68	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	A	67	ARG	NE-CZ-NH2	-13.63	113.49	120.30
1	A	376	GLY	O-C-N	-13.36	101.33	122.70
1	B	104	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	B	371	PHE	CB-CG-CD2	12.07	129.25	120.80
1	A	255	ASP	CB-CG-OD2	11.98	129.08	118.30
1	A	328	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	B	156	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	A	350	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	B	380	GLU	OE1-CD-OE2	-11.38	109.65	123.30
1	B	160	TYR	CB-CG-CD2	-10.97	114.42	121.00
1	B	61	ASP	CB-CG-OD2	-10.79	108.59	118.30
1	A	348	GLU	OE1-CD-OE2	-10.74	110.41	123.30
1	A	233	GLU	OE1-CD-OE2	10.70	136.14	123.30
1	B	376	GLY	CA-C-N	10.68	140.69	117.20
1	B	8	ARG	NH1-CZ-NH2	10.66	131.13	119.40
1	B	227	ASP	CB-CG-OD1	10.55	127.80	118.30
1	B	199	ARG	NE-CZ-NH2	10.53	125.56	120.30
1	A	156	ARG	NE-CZ-NH1	-10.52	115.04	120.30
1	B	294	ASP	CB-CG-OD2	-10.50	108.85	118.30
1	A	101	GLU	OE1-CD-OE2	-10.43	110.78	123.30
1	A	12	ARG	CD-NE-CZ	10.00	137.60	123.60
1	B	259	ARG	NH1-CZ-NH2	-9.96	108.44	119.40
1	B	385	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	A	92	ASP	CB-CG-OD1	-9.85	109.43	118.30
1	B	69	TYR	CB-CG-CD2	-9.79	115.13	121.00
1	A	12	ARG	NH1-CZ-NH2	9.78	130.15	119.40
1	A	199	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	B	56	PHE	CB-CG-CD2	9.55	127.48	120.80
1	A	61	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	B	388	ALA	C-N-CA	9.49	145.43	121.70
1	B	137	MET	CA-C-O	-9.38	100.39	120.10
1	B	141	ASP	CB-CG-OD1	9.37	126.73	118.30
1	A	342	VAL	CG1-CB-CG2	9.35	125.86	110.90
1	B	265	PHE	CB-CG-CD1	-9.34	114.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ARG	NH1-CZ-NH2	9.30	129.63	119.40
1	A	344	PHE	CB-CG-CD1	9.16	127.21	120.80
1	B	141	ASP	CB-CG-OD2	9.16	126.55	118.30
1	B	176	ASP	CB-CG-OD1	9.12	126.51	118.30
1	B	311	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	207	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	B	160	TYR	CB-CG-CD1	9.04	126.43	121.00
1	B	376	GLY	CA-C-O	-9.01	104.39	120.60
1	A	376	GLY	N-CA-C	-8.93	90.78	113.10
1	B	207	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	185	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	B	168	GLY	O-C-N	-8.80	108.62	122.70
1	A	388	ALA	N-CA-CB	8.75	122.34	110.10
1	B	141	ASP	OD1-CG-OD2	-8.74	106.69	123.30
1	B	350	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	B	92	ASP	CB-CG-OD2	8.66	126.09	118.30
1	A	328	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	A	138	PRO	N-CA-CB	8.58	113.59	103.30
1	B	284	VAL	CA-CB-CG1	8.30	123.35	110.90
1	B	96	ASP	CB-CG-OD2	8.23	125.71	118.30
1	A	157	TYR	CB-CG-CD2	8.21	125.93	121.00
1	B	249	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	333	GLU	OE1-CD-OE2	-8.08	113.60	123.30
1	A	157	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	A	156	ARG	NH1-CZ-NH2	7.96	128.15	119.40
1	B	259	ARG	NE-CZ-NH2	7.93	124.27	120.30
1	A	198	PHE	CB-CG-CD1	7.88	126.32	120.80
1	B	172	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	86	TYR	CB-CG-CD1	-7.87	116.28	121.00
1	B	259	ARG	CD-NE-CZ	7.86	134.60	123.60
1	A	270	ASP	CB-CG-OD1	7.85	125.36	118.30
1	B	56	PHE	CB-CG-CD1	-7.80	115.34	120.80
1	B	265	PHE	CB-CG-CD2	7.75	126.22	120.80
1	B	317	LEU	O-C-N	7.69	135.01	122.70
1	A	172	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	A	8	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	A	94	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	A	92	ASP	OD1-CG-OD2	7.53	137.61	123.30
1	A	253	ALA	N-CA-CB	7.49	120.59	110.10
1	B	8	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	B	14	GLU	OE1-CD-OE2	-7.44	114.38	123.30
1	A	104	ARG	NE-CZ-NH1	7.34	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	A	141	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	B	342	VAL	N-CA-CB	-7.25	95.56	111.50
1	B	371	PHE	CB-CG-CD1	-7.23	115.74	120.80
1	A	203	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	156	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	116	GLU	OE1-CD-OE2	-7.13	114.74	123.30
1	B	347	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	328	ARG	CD-NE-CZ	7.10	133.54	123.60
1	B	137	MET	CG-SD-CE	-7.05	88.92	100.20
1	B	342	VAL	CB-CA-C	7.01	124.72	111.40
1	B	314	GLU	OE1-CD-OE2	7.01	131.71	123.30
1	A	137	MET	CA-C-O	-7.00	105.39	120.10
1	B	196	VAL	CG1-CB-CG2	-7.00	99.71	110.90
1	B	342	VAL	CA-CB-CG2	6.90	121.25	110.90
1	A	334	TYR	CB-CG-CD1	6.86	125.12	121.00
1	B	315	GLN	O-C-N	-6.84	111.75	122.70
1	A	219	ALA	N-CA-CB	6.84	119.67	110.10
1	B	86	TYR	CA-CB-CG	-6.82	100.44	113.40
1	A	38	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	199	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
1	B	172	ARG	NH1-CZ-NH2	-6.79	111.93	119.40
1	B	317	LEU	CA-C-O	-6.71	106.00	120.10
1	A	389	ILE	CA-CB-CG2	6.71	124.33	110.90
1	A	273	GLY	CA-C-O	-6.65	108.64	120.60
1	A	138	PRO	CA-N-CD	-6.64	102.21	111.50
1	A	86	TYR	CB-CG-CD2	6.63	124.98	121.00
1	A	160	TYR	CB-CG-CD2	6.57	124.94	121.00
1	A	56	PHE	CB-CG-CD2	-6.55	116.21	120.80
1	A	160	TYR	CB-CG-CD1	-6.53	117.08	121.00
1	B	92	ASP	CA-C-O	-6.52	106.40	120.10
1	B	385	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
1	B	328	ARG	CD-NE-CZ	6.42	132.58	123.60
1	B	156	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	B	186	VAL	CA-CB-CG1	6.40	120.50	110.90
1	B	142	TYR	CB-CG-CD1	6.38	124.83	121.00
1	B	151	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	A	8	ARG	NH1-CZ-NH2	-6.36	112.41	119.40
1	A	259	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	294	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	137	MET	CG-SD-CE	-6.28	90.16	100.20
1	B	104	ARG	CD-NE-CZ	6.28	132.39	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	108	GLU	OE1-CD-OE2	-6.25	115.79	123.30
1	B	45	ASN	OD1-CG-ND2	6.23	136.22	121.90
1	B	142	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	B	94	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	142	TYR	CA-C-O	-6.14	107.21	120.10
1	A	8	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	363	GLU	O-C-N	-6.11	112.82	123.20
1	B	12	ARG	N-CA-CB	-6.10	99.61	110.60
1	A	227	ASP	CA-C-O	6.10	132.91	120.10
1	B	175	LYS	CA-C-O	6.09	132.90	120.10
1	B	116	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	B	168	GLY	CA-C-O	5.99	131.38	120.60
1	B	255	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	B	244	GLN	CG-CD-NE2	5.96	131.01	116.70
1	B	322	GLU	OE1-CD-OE2	5.96	130.46	123.30
1	A	140	ALA	N-CA-CB	5.95	118.42	110.10
1	A	207	ASP	OD1-CG-OD2	5.94	134.59	123.30
1	A	92	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	54	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	B	74	GLU	CA-C-N	5.93	130.25	117.20
1	A	260	GLU	OE1-CD-OE2	5.92	130.41	123.30
1	B	233	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	A	342	VAL	N-CA-CB	-5.92	98.48	111.50
1	A	104	ARG	CD-NE-CZ	5.92	131.88	123.60
1	B	112	LYS	CA-C-O	5.91	132.50	120.10
1	B	185	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
1	B	187	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	A	29	ASN	CA-C-O	5.87	132.43	120.10
1	B	12	ARG	CD-NE-CZ	5.86	131.81	123.60
1	A	79	GLU	CB-CA-C	-5.86	98.68	110.40
1	B	371	PHE	CG-CD2-CE2	5.86	127.25	120.80
1	B	175	LYS	O-C-N	-5.80	113.41	122.70
1	B	372	GLY	CA-C-N	5.79	129.93	117.20
1	A	292	ILE	CA-CB-CG2	5.78	122.47	110.90
1	B	340	ALA	N-CA-CB	-5.76	102.03	110.10
1	A	334	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	344	PHE	CB-CG-CD2	-5.75	116.78	120.80
1	A	388	ALA	CA-C-O	5.75	132.16	120.10
1	A	303	HIS	CA-CB-CG	-5.74	103.83	113.60
1	B	277	LYS	CB-CA-C	-5.74	98.92	110.40
1	A	389	ILE	CB-CA-C	5.74	123.07	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	92	ASP	O-C-N	5.71	131.84	122.70
1	A	68	ARG	NH1-CZ-NH2	5.69	125.66	119.40
1	B	14	GLU	CA-C-O	-5.68	108.17	120.10
1	B	377	LEU	CB-CG-CD2	-5.68	101.35	111.00
1	B	14	GLU	CA-C-N	5.67	127.55	116.20
1	A	132	THR	CA-CB-CG2	5.66	120.32	112.40
1	A	251	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	A	313	VAL	CA-C-O	5.65	131.97	120.10
1	A	329	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	148	LEU	CA-C-N	5.64	127.49	116.20
1	A	71	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	282	ALA	CA-C-O	5.63	131.93	120.10
1	A	377	LEU	N-CA-CB	5.62	121.64	110.40
1	B	192	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	B	150	LEU	O-C-N	-5.61	113.72	122.70
1	A	153	TYR	CB-CG-CD1	-5.61	117.64	121.00
1	B	80	ASN	CB-CG-ND2	5.60	130.15	116.70
1	A	58	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	B	79	GLU	O-C-N	-5.58	113.78	122.70
1	A	136	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	69	TYR	CA-CB-CG	-5.57	102.83	113.40
1	A	99	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	B	203	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	278	ASN	CB-CG-ND2	5.55	130.01	116.70
1	B	227	ASP	OD1-CG-OD2	-5.54	112.78	123.30
1	B	92	ASP	OD1-CG-OD2	-5.53	112.79	123.30
1	B	265	PHE	O-C-N	-5.53	113.85	122.70
1	A	141	ASP	OD1-CG-OD2	5.53	133.80	123.30
1	A	172	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	B	69	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	334	TYR	CA-C-O	-5.52	108.51	120.10
1	B	135	VAL	CA-CB-CG1	5.51	119.16	110.90
1	A	233	GLU	CG-CD-OE2	-5.50	107.30	118.30
1	A	111	VAL	O-C-N	-5.49	113.92	122.70
1	B	151	ARG	NH1-CZ-NH2	5.48	125.43	119.40
1	B	61	ASP	OD1-CG-OD2	5.48	133.71	123.30
1	A	362	GLY	CA-C-O	5.47	130.45	120.60
1	A	66	LYS	CB-CA-C	-5.47	99.47	110.40
1	A	205	HIS	CA-C-O	5.46	131.57	120.10
1	B	296	ASN	O-C-N	-5.46	113.96	122.70
1	A	381	THR	OG1-CB-CG2	-5.46	97.44	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	GLU	O-C-N	5.44	131.41	122.70
1	A	322	GLU	CB-CA-C	-5.44	99.52	110.40
1	B	119	GLN	CG-CD-OE1	-5.44	110.72	121.60
1	B	328	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	337	MET	O-C-N	-5.42	114.02	122.70
1	B	325	ASN	O-C-N	-5.42	114.03	122.70
1	B	93	ALA	N-CA-CB	-5.42	102.51	110.10
1	B	319	LEU	CA-C-O	-5.42	108.72	120.10
1	B	261	ALA	N-CA-CB	-5.40	102.54	110.10
1	A	334	TYR	O-C-N	5.39	132.37	123.20
1	A	376	GLY	CA-C-O	-5.39	110.90	120.60
1	B	206	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	81	PRO	O-C-N	-5.39	114.08	122.70
1	A	205	HIS	O-C-N	-5.38	114.08	122.70
1	A	217	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	B	329	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	B	167	GLY	N-CA-C	-5.36	99.71	113.10
1	B	176	ASP	OD1-CG-OD2	-5.35	113.13	123.30
1	A	226	SER	O-C-N	-5.35	114.14	122.70
1	B	336	ASN	OD1-CG-ND2	-5.33	109.65	121.90
1	B	206	LEU	CA-C-O	5.32	131.27	120.10
1	B	220	ALA	O-C-N	-5.31	114.20	122.70
1	B	172	ARG	O-C-N	-5.30	114.22	122.70
1	A	331	LEU	CA-C-O	5.30	131.22	120.10
1	B	252	GLY	CA-C-O	-5.29	111.08	120.60
1	A	111	VAL	CA-C-O	5.29	131.21	120.10
1	A	56	PHE	CA-C-O	5.28	131.19	120.10
1	B	65	ILE	O-C-N	5.28	131.15	122.70
1	B	128	ILE	O-C-N	5.26	131.12	122.70
1	B	62	LYS	CA-CB-CG	5.26	124.96	113.40
1	A	312	GLN	CB-CA-C	5.25	120.90	110.40
1	B	34	SER	CA-C-N	5.24	128.74	117.20
1	B	255	ASP	OD1-CG-OD2	5.24	133.26	123.30
1	B	146	LYS	CA-CB-CG	5.24	124.93	113.40
1	A	154	VAL	CA-CB-CG1	5.23	118.74	110.90
1	B	21	ALA	N-CA-CB	-5.22	102.79	110.10
1	B	328	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	288	GLU	N-CA-CB	5.22	120.00	110.60
1	B	138	PRO	N-CA-CB	5.20	109.54	103.30
1	B	190	CYS	O-C-N	5.20	131.02	122.70
1	B	255	ASP	N-CA-CB	5.20	119.95	110.60
1	B	253	ALA	N-CA-CB	-5.20	102.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	B	385	ARG	CA-C-O	-5.19	109.21	120.10
1	B	319	LEU	O-C-N	5.18	130.99	122.70
1	B	329	GLU	CA-C-O	5.18	130.98	120.10
1	A	41	PHE	CB-CG-CD2	5.18	124.43	120.80
1	B	273	GLY	O-C-N	-5.18	114.42	122.70
1	B	260	GLU	N-CA-CB	-5.17	101.29	110.60
1	B	87	MET	CA-CB-CG	5.17	122.09	113.30
1	A	107	LYS	O-C-N	-5.17	114.44	122.70
1	A	168	GLY	CA-C-O	-5.16	111.31	120.60
1	A	359	LYS	CA-C-O	-5.14	109.30	120.10
1	B	86	TYR	CA-C-O	5.14	130.90	120.10
1	A	104	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	B	166	ALA	CA-C-O	-5.13	109.33	120.10
1	B	255	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	B	367	TRP	CB-CG-CD2	-5.13	119.93	126.60
1	A	351	LYS	O-C-N	-5.13	114.50	122.70
1	B	65	ILE	CA-C-O	-5.13	109.33	120.10
1	A	199	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	A	49	LYS	O-C-N	-5.12	114.51	122.70
1	A	212	GLN	O-C-N	-5.11	114.52	122.70
1	B	212	GLN	CG-CD-OE1	5.11	131.82	121.60
1	B	105	LEU	CA-C-O	5.10	130.81	120.10
1	B	12	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	234	LYS	N-CA-CB	-5.09	101.44	110.60
1	A	196	VAL	CA-CB-CG1	5.08	118.53	110.90
1	B	311	ASP	OD1-CG-OD2	5.08	132.95	123.30
1	A	381	THR	O-C-N	-5.06	114.61	122.70
1	B	35	THR	O-C-N	-5.06	114.61	122.70
1	B	85	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	B	52	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	260	GLU	CG-CD-OE1	5.03	128.35	118.30
1	A	171	LEU	O-C-N	5.01	130.72	122.70
1	B	30	CYS	CA-C-O	5.00	130.61	120.10
1	B	270	ASP	CB-CG-OD1	5.00	122.80	118.30

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	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	A	166	ALA	Mainchain
1	A	248	PRO	Mainchain
1	A	337	MET	Mainchain
1	A	376	GLY	Peptide,Mainchain
1	A	56	PHE	Mainchain
1	B	118	GLY	Mainchain
1	B	137	MET	Peptide,Mainchain
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	Peptide,Mainchain

## 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	49	1
1	B	2995	0	3042	59	1
2	A	103	0	61	13	0
2	B	103	0	61	13	0
3	A	232	0	0	4	7
3	B	208	0	0	7	6
All	All	6636	0	6207	116	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 9.

All (116) 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: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:A:59:MET:HE2	2:A:390[B]:HXC:H1'	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:MET:HE2	2:B:391[B]:HXC:H1'	1.82	0.60
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
1:B:93:ALA:O	1:B:97:MET:HG3	2.03	0.58
1:B:59:MET:CE	2:B:391[B]:HXC:H1'	2.33	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:377:LEU:C	1:A:377:LEU:HD23	2.35	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:59:MET:CE	2:A:390[B]:HXC:H1'	2.41	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:49:LYS:HB2	3:B:463:HOH:O	2.15	0.46
1:B:377:LEU:HD23	1:B:377:LEU:C	2.37	0.45
1:B:90:SER:O	1:B:94:ARG:HG3	2.17	0.45
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:54:GLU:HB3	1:B:58:ARG:HH12	1.82	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:159:MET:HB3	1:B:162:GLN:CD	2.38	0.43
1:B:24:THR:HB	1:B:344:PHE:CZ	2.53	0.43
1:A:87:MET:HE1	1:A:264:THR:HG21	1.99	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:O	1:B:91:LEU:HG	2.20	0.41
1:B:42:LYS:HG3	1:B:47:GLU:CD	2.41	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:78:LYS:HG2	1:B:79:GLU:N	2.36	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
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%)	29 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	387/389 (100%)	370 (96%)	16 (4%)	1 (0%)	41	31
All	All	774/778 (100%)	746 (96%)	25 (3%)	3 (0%)	34	24

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/325 (100%)	314 (97%)	11 (3%)	37	28
1	B	325/325 (100%)	311 (96%)	14 (4%)	29	19
All	All	650/650 (100%)	625 (96%)	25 (4%)	33	24

All (25) 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	133	SER
1	A	235	PRO
1	A	268	LEU
1	A	279	ILE
1	A	284	VAL
1	A	292	ILE
1	A	342	VAL
1	A	350	ARG
1	B	1	MET
1	B	45	ASN

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Mol	Chain	Res	Type
1	B	46	SER
1	B	50	THR
1	B	58	ARG
1	B	62	LYS
1	B	67	ARG
1	B	78	LYS
1	B	160	TYR
1	B	255	ASP
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	A	315	GLN
1	B	303	HIS
1	B	312	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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]	-	49,57,57	15.56	9 (18%)	60,83,83	7.38	19 (31%)
2	HXC	A	390[A]	-	49,57,57	14.08	9 (18%)	60,83,83	6.83	22 (36%)
2	HXC	A	390[B]	-	49,57,57	1.80	10 (20%)	60,83,83	3.23	29 (48%)
2	HXC	B	391[B]	-	49,57,57	1.99	9 (18%)	60,83,83	3.65	30 (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
2	HXC	B	391[A]	-	-	17/52/72/72	0/3/3/3
2	HXC	A	390[A]	-	-	12/52/72/72	0/3/3/3
2	HXC	A	390[B]	-	-	18/52/72/72	0/3/3/3
2	HXC	B	391[B]	-	-	21/52/72/72	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391[A]	HXC	CM1-S	108.30	4.39	1.76
2	A	390[A]	HXC	CM1-S	97.86	4.14	1.76
2	B	391[A]	HXC	CM3-CM2	-7.41	1.24	1.52
2	B	391[B]	HXC	CM3-CM2	-7.41	1.24	1.52
2	A	390[A]	HXC	CM3-CM2	-7.00	1.26	1.52
2	A	390[B]	HXC	CM3-CM2	-7.00	1.26	1.52
2	A	390[B]	HXC	CP2-NP1	4.89	1.57	1.46
2	B	391[B]	HXC	CP2-NP1	4.64	1.56	1.46
2	B	391[B]	HXC	CM1-S	4.24	1.86	1.76
2	B	391[B]	HXC	CP5-NP2	4.05	1.55	1.46
2	A	390[A]	HXC	CP2-NP1	3.93	1.55	1.46
2	B	391[B]	HXC	C2-N3	-3.87	1.25	1.32
2	B	391[A]	HXC	CM2-CM1	3.78	1.54	1.50
2	B	391[B]	HXC	CM2-CM1	3.78	1.54	1.50
2	B	391[B]	HXC	P3-O33	3.70	1.62	1.50
2	A	390[B]	HXC	P3-O33	3.39	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	3.35	1.84	1.76
2	B	391[A]	HXC	CP5-NP2	3.23	1.53	1.46
2	B	391[A]	HXC	P2-O7	-3.02	1.47	1.59
2	B	391[A]	HXC	P3-O33	2.97	1.60	1.50
2	B	391[B]	HXC	P2-O7	-2.81	1.47	1.59
2	A	390[A]	HXC	P3-O33	2.79	1.59	1.50
2	A	390[A]	HXC	P2-O7	-2.76	1.48	1.59
2	A	390[B]	HXC	C2'-C1'	-2.76	1.49	1.53
2	A	390[A]	HXC	CM2-CM1	2.65	1.53	1.50
2	A	390[B]	HXC	CM2-CM1	2.65	1.53	1.50
2	A	390[A]	HXC	CP5-NP2	2.60	1.52	1.46
2	A	390[B]	HXC	P2-O7	-2.56	1.48	1.59
2	A	390[B]	HXC	CP5-NP2	2.56	1.52	1.46
2	B	391[A]	HXC	CP2-NP1	2.41	1.51	1.46
2	A	390[B]	HXC	CP1-S	2.31	1.91	1.81
2	A	390[A]	HXC	C2-N1	2.28	1.38	1.33
2	A	390[A]	HXC	OM2-CM1	2.13	1.24	1.21
2	A	390[B]	HXC	OM2-CM1	2.13	1.24	1.21
2	B	391[B]	HXC	O4'-C1'	-2.10	1.38	1.41
2	B	391[A]	HXC	C2'-C1'	-2.06	1.50	1.53
2	B	391[A]	HXC	P3-O32	-2.03	1.47	1.54

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391[A]	HXC	OM2-CM1-S	-30.59	82.88	122.61
2	B	391[A]	HXC	O4'-C4'-C3'	-26.63	47.80	104.87
2	A	390[A]	HXC	O32-P3-O33	-26.44	7.16	110.68
2	A	390[A]	HXC	OM2-CM1-S	-25.99	88.85	122.61
2	B	391[A]	HXC	CP1-S-CM1	-24.26	26.34	101.87
2	B	391[A]	HXC	CM2-CM1-S	-23.40	86.22	113.46
2	A	390[A]	HXC	CM2-CM1-S	-19.18	91.13	113.46
2	A	390[A]	HXC	C2'-C3'-C4'	-14.92	76.78	103.22
2	A	390[A]	HXC	CP1-S-CM1	-14.84	55.67	101.87
2	A	390[A]	HXC	O4'-C1'-C2'	-12.77	88.27	106.93
2	B	391[A]	HXC	O4'-C1'-C2'	-12.26	89.01	106.93
2	A	390[A]	HXC	C3'-C2'-C1'	10.76	123.72	99.89
2	B	391[A]	HXC	C3'-C2'-C1'	-10.36	76.94	99.89
2	B	391[B]	HXC	CP4-CP3-NP1	10.01	133.27	116.42
2	B	391[B]	HXC	OP1-CP3-NP1	-9.66	104.78	123.01
2	A	390[B]	HXC	OP1-CP3-NP1	-8.87	106.28	123.01
2	B	391[B]	HXC	CM2-CM1-S	-8.74	103.28	113.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391[B]	HXC	OM2-CM1-S	7.96	132.95	122.61
2	B	391[A]	HXC	CM3-CM2-CM1	7.71	129.44	112.33
2	B	391[B]	HXC	CM3-CM2-CM1	7.71	129.44	112.33
2	A	390[B]	HXC	O2'-C2'-C1'	7.63	139.02	110.85
2	A	390[B]	HXC	C5-C6-N1	-7.60	103.12	120.35
2	A	390[B]	HXC	CP4-CP3-NP1	7.52	129.07	116.42
2	A	390[A]	HXC	CP2-NP1-CP3	-7.02	109.80	122.84
2	A	390[B]	HXC	CP5-NP2-CP6	-6.77	110.51	122.59
2	A	390[B]	HXC	CM2-CM1-S	-6.74	105.61	113.46
2	B	391[B]	HXC	O7-CPB-CPA	-6.44	100.19	110.55
2	B	391[B]	HXC	CP5-NP2-CP6	-6.24	111.45	122.59
2	B	391[B]	HXC	O2'-C2'-C1'	6.22	133.81	110.85
2	A	390[A]	HXC	OP1-CP3-NP1	-6.03	111.64	123.01
2	A	390[A]	HXC	CP4-CP3-NP1	5.66	125.96	116.42
2	A	390[A]	HXC	CP9-CPA-CP7	5.64	118.61	108.82
2	A	390[A]	HXC	O3'-C3'-C4'	5.35	129.44	110.08
2	B	391[B]	HXC	CP5-CP4-CP3	5.05	120.77	112.36
2	B	391[B]	HXC	C5-C6-N1	-4.95	109.12	120.35
2	A	390[A]	HXC	CM3-CM2-CM1	4.84	123.06	112.33
2	A	390[B]	HXC	CM3-CM2-CM1	4.84	123.06	112.33
2	A	390[B]	HXC	O4'-C4'-C3'	4.82	115.20	104.87
2	B	391[A]	HXC	CP2-NP1-CP3	-4.79	113.95	122.84
2	B	391[B]	HXC	C4-C5-N7	4.78	114.38	109.40
2	A	390[B]	HXC	O7-CPB-CPA	-4.75	102.91	110.55
2	B	391[B]	HXC	C2'-C3'-C4'	-4.73	94.85	103.22
2	A	390[B]	HXC	C2'-C3'-C4'	-4.65	94.98	103.22
2	B	391[B]	HXC	O4'-C4'-C3'	4.50	114.51	104.87
2	B	391[A]	HXC	OP3-CP7-CP6	-4.27	88.86	109.42
2	A	390[A]	HXC	CP5-NP2-CP6	-4.19	115.11	122.59
2	A	390[A]	HXC	OM2-CM1-CM2	4.05	128.77	123.99
2	A	390[B]	HXC	OM2-CM1-CM2	4.05	128.77	123.99
2	B	391[A]	HXC	O3'-C3'-C4'	4.01	124.58	110.08
2	A	390[A]	HXC	C1'-N9-C4	3.91	133.51	126.64
2	A	390[B]	HXC	C5-C6-N6	-3.90	114.43	120.35
2	A	390[A]	HXC	C5-C6-N6	3.84	126.19	120.35
2	A	390[B]	HXC	CP9-CPA-CP7	3.82	115.44	108.82
2	B	391[B]	HXC	N3-C2-N1	3.79	134.60	128.68
2	B	391[A]	HXC	CM4-CM3-CM2	3.78	126.79	113.19
2	B	391[B]	HXC	CM4-CM3-CM2	3.78	126.79	113.19
2	B	391[B]	HXC	N6-C6-N1	3.72	126.30	118.57
2	B	391[A]	HXC	CM5-CM4-CM3	3.59	148.66	115.30
2	B	391[B]	HXC	CM5-CM4-CM3	3.59	148.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390[B]	HXC	C4-C5-N7	3.47	113.02	109.40
2	B	391[B]	HXC	CP9-CPA-CP7	3.45	114.80	108.82
2	B	391[A]	HXC	CP9-CPA-CPB	3.35	113.70	108.23
2	A	390[B]	HXC	OP2-CP6-NP2	-3.34	115.83	122.99
2	A	390[B]	HXC	CP2-NP1-CP3	-3.16	116.96	122.84
2	A	390[B]	HXC	O3'-C3'-C4'	3.09	121.27	110.08
2	A	390[B]	HXC	CP4-CP5-NP2	2.97	117.88	111.90
2	A	390[B]	HXC	C1'-N9-C4	2.96	131.85	126.64
2	B	391[A]	HXC	CP9-CPA-CP7	-2.89	103.81	108.82
2	B	391[B]	HXC	C1'-N9-C4	2.86	131.67	126.64
2	B	391[B]	HXC	O3'-C3'-C4'	2.84	120.34	110.08
2	A	390[B]	HXC	C3'-C2'-C1'	2.81	106.12	99.89
2	A	390[B]	HXC	CP1-CP2-NP1	2.77	118.23	112.42
2	B	391[B]	HXC	C3'-C2'-C1'	2.69	105.85	99.89
2	B	391[B]	HXC	C5-C6-N6	2.68	124.43	120.35
2	A	390[A]	HXC	CM5-CM4-CM3	2.60	139.46	115.30
2	A	390[B]	HXC	CM5-CM4-CM3	2.60	139.46	115.30
2	A	390[A]	HXC	CP1-CP2-NP1	-2.57	107.02	112.42
2	B	391[A]	HXC	C5-C6-N6	2.55	124.22	120.35
2	B	391[B]	HXC	P2-O6-P1	2.51	141.43	132.83
2	B	391[B]	HXC	O32-P3-O33	-2.48	100.96	110.68
2	A	390[B]	HXC	CP9-CPA-CPB	-2.47	104.20	108.23
2	A	390[B]	HXC	N3-C2-N1	2.42	132.46	128.68
2	B	391[B]	HXC	OP2-CP6-NP2	-2.41	117.82	122.99
2	A	390[B]	HXC	O3'-C3'-C2'	2.40	120.38	111.68
2	A	390[B]	HXC	O32-P3-O33	-2.38	101.36	110.68
2	B	391[B]	HXC	O4'-C1'-C2'	-2.38	103.45	106.93
2	B	391[A]	HXC	O7-CPB-CPA	-2.37	106.73	110.55
2	B	391[A]	HXC	C4-C5-N7	2.36	111.86	109.40
2	A	390[A]	HXC	O2'-C2'-C3'	-2.29	104.65	111.17
2	A	390[A]	HXC	O3'-P3-O33	-2.28	100.58	109.39
2	B	391[A]	HXC	CP5-NP2-CP6	-2.27	118.53	122.59
2	B	391[B]	HXC	CP1-CP2-NP1	2.26	117.16	112.42
2	B	391[A]	HXC	O3'-P3-O33	-2.25	100.69	109.39
2	A	390[B]	HXC	CP7-CP6-NP2	2.25	121.06	116.58
2	B	391[B]	HXC	O3'-C3'-C2'	2.19	119.60	111.68
2	B	391[B]	HXC	CP2-NP1-CP3	-2.14	118.86	122.84
2	A	390[B]	HXC	P1-O5'-C5'	2.09	133.94	121.68
2	A	390[A]	HXC	OP2-CP6-NP2	2.06	127.43	122.99
2	A	390[B]	HXC	P2-O6-P1	2.05	139.87	132.83
2	B	391[B]	HXC	CP7-CP6-NP2	2.01	120.57	116.58

There are no chirality outliers.



All (68) 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	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	C3'-O3'-P3-O33
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	OP1-CP3-CP4-CP5
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	C3'-O3'-P3-O33
2	B	391[A]	HXC	C5'-O5'-P1-O11
2	B	391[A]	HXC	C5'-O5'-P1-O12
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	C3'-O3'-P3-O33
2	B	391[B]	HXC	CPB-O7-P2-O6
2	B	391[B]	HXC	CP7-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[A]	HXC	C2'-C3'-O3'-P3
2	B	391[A]	HXC	C2'-C3'-O3'-P3
2	B	391[A]	HXC	CM2-CM3-CM4-CM5
2	B	391[B]	HXC	CM2-CM3-CM4-CM5
2	B	391[A]	HXC	S-CP1-CP2-NP1
2	B	391[A]	HXC	CM3-CM4-CM5-CM6
2	B	391[B]	HXC	CM3-CM4-CM5-CM6
2	B	391[B]	HXC	CP9-CPA-CPB-O7
2	B	391[B]	HXC	CP8-CPA-CPB-O7
2	B	391[B]	HXC	S-CP1-CP2-NP1

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Mol	Chain	Res	Type	Atoms
2	A	390[B]	HXC	CP1-CP2-NP1-CP3
2	B	391[B]	HXC	OP2-CP6-NP2-CP5
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-O31
2	A	390[B]	HXC	C5'-O5'-P1-O6
2	B	391[A]	HXC	C3'-O3'-P3-O31
2	B	391[B]	HXC	C3'-O3'-P3-O31
2	A	390[A]	HXC	C5'-O5'-P1-O11
2	A	390[B]	HXC	C5'-O5'-P1-O12
2	B	391[B]	HXC	CPB-O7-P2-O21
2	A	390[B]	HXC	OP1-CP3-NP1-CP2
2	B	391[B]	HXC	OP1-CP3-CP4-CP5
2	A	390[B]	HXC	S-CP1-CP2-NP1
2	B	391[A]	HXC	C3'-C4'-C5'-O5'
2	A	390[A]	HXC	C3'-O3'-P3-O33
2	B	391[B]	HXC	CP1-CP2-NP1-CP3
2	A	390[A]	HXC	C3'-O3'-P3-O31
2	A	390[A]	HXC	C5'-O5'-P1-O6
2	A	390[B]	HXC	NP1-CP3-CP4-CP5
2	B	391[A]	HXC	C5'-O5'-P1-O6
2	A	390[B]	HXC	O4'-C4'-C5'-O5'
2	B	391[B]	HXC	P1-O6-P2-O22
2	B	391[B]	HXC	CPB-O7-P2-O22
2	A	390[A]	HXC	NP1-CP3-CP4-CP5
2	B	391[B]	HXC	NP1-CP3-CP4-CP5

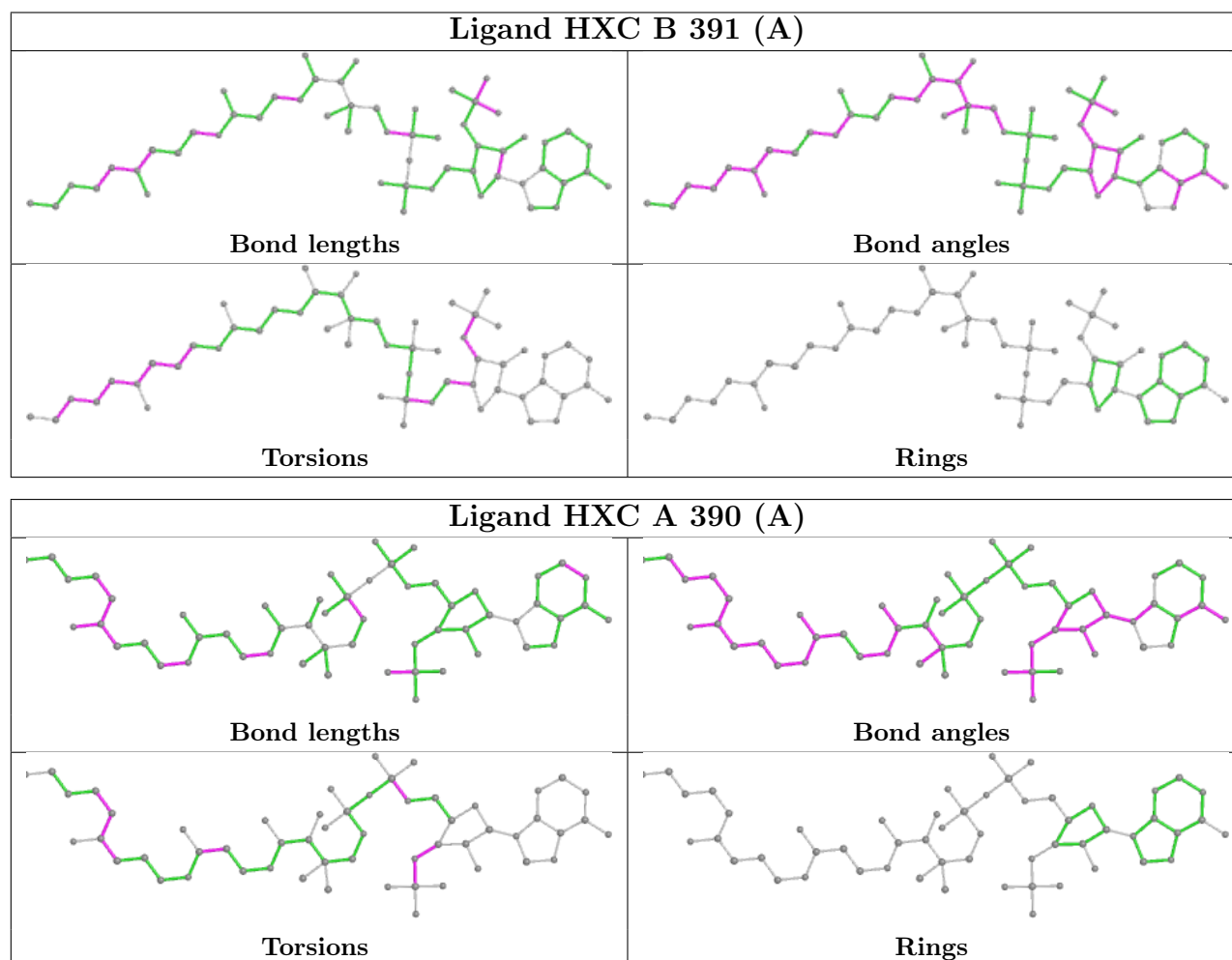
There are no ring outliers.

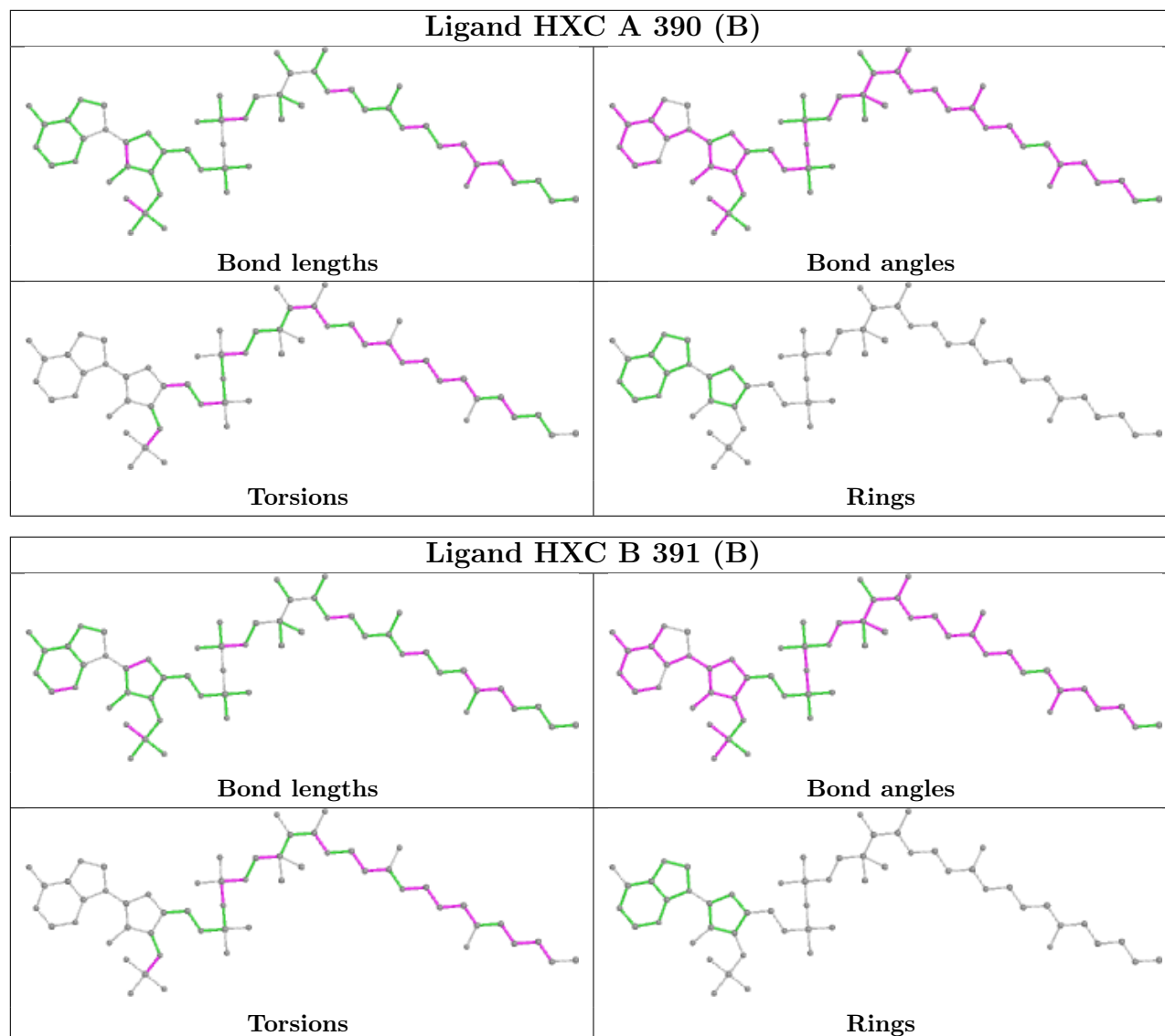
4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	391[A]	HXC	5	0
2	A	390[A]	HXC	3	0
2	A	390[B]	HXC	10	0
2	B	391[B]	HXC	8	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/389 (100%)	-0.20	6 (1%) 73 76	11, 20, 36, 63	0
1	B	389/389 (100%)	-0.11	9 (2%) 60 63	11, 21, 43, 71	0
All	All	778/778 (100%)	-0.16	15 (1%) 66 69	11, 20, 39, 71	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.4
1	B	1	MET	4.9
1	B	231	GLU	3.8
1	A	215	PHE	3.2
1	A	231	GLU	3.0
1	A	2	VAL	2.8
1	B	42	LYS	2.7
1	B	48	HIS	2.7
1	A	389	ILE	2.5
1	B	39	PHE	2.3
1	B	215	PHE	2.2
1	A	268	LEU	2.2
1	B	47	GLU	2.2
1	B	78	LYS	2.1
1	B	45	ASN	2.1

### 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](#)

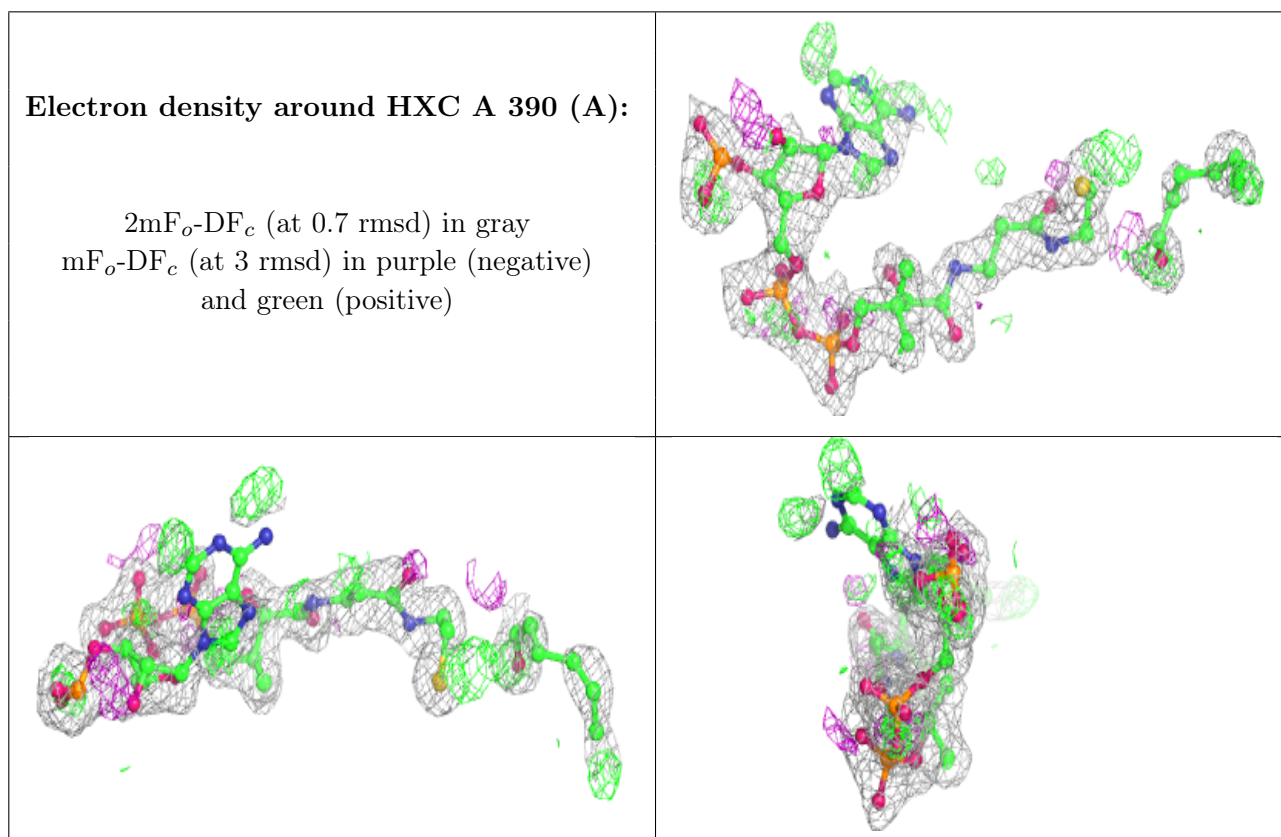
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

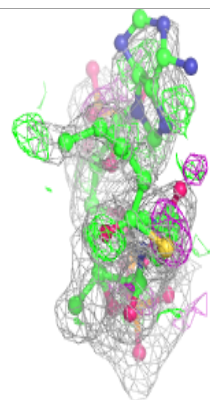
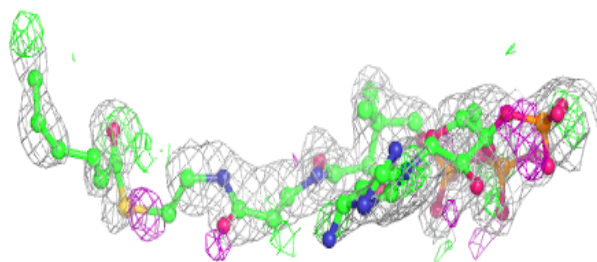
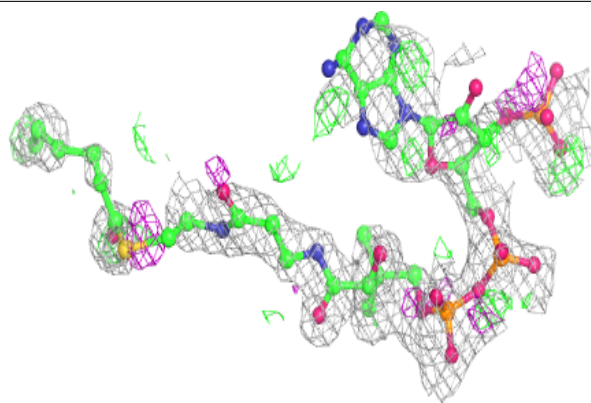
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HXC	A	390[A]	55/55	0.74	0.27	6,41,85,86	52
2	HXC	A	390[B]	55/55	0.74	0.27	6,58,75,76	52
2	HXC	B	391[A]	55/55	0.77	0.26	7,45,86,87	52
2	HXC	B	391[B]	55/55	0.77	0.26	7,55,75,75	52

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.

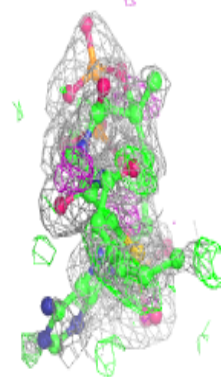
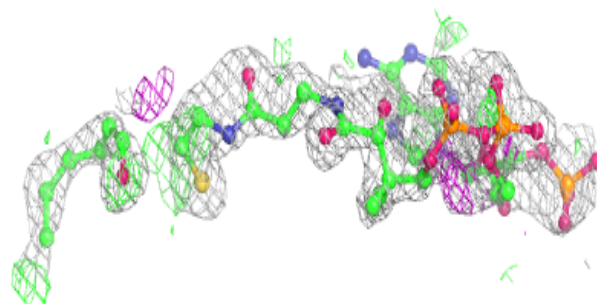
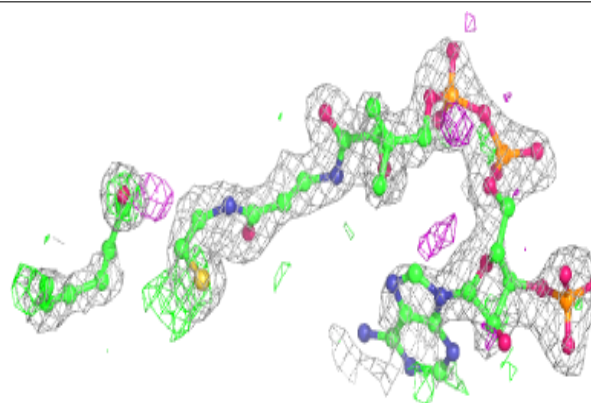


**Electron density around HXC A 390 (B):**

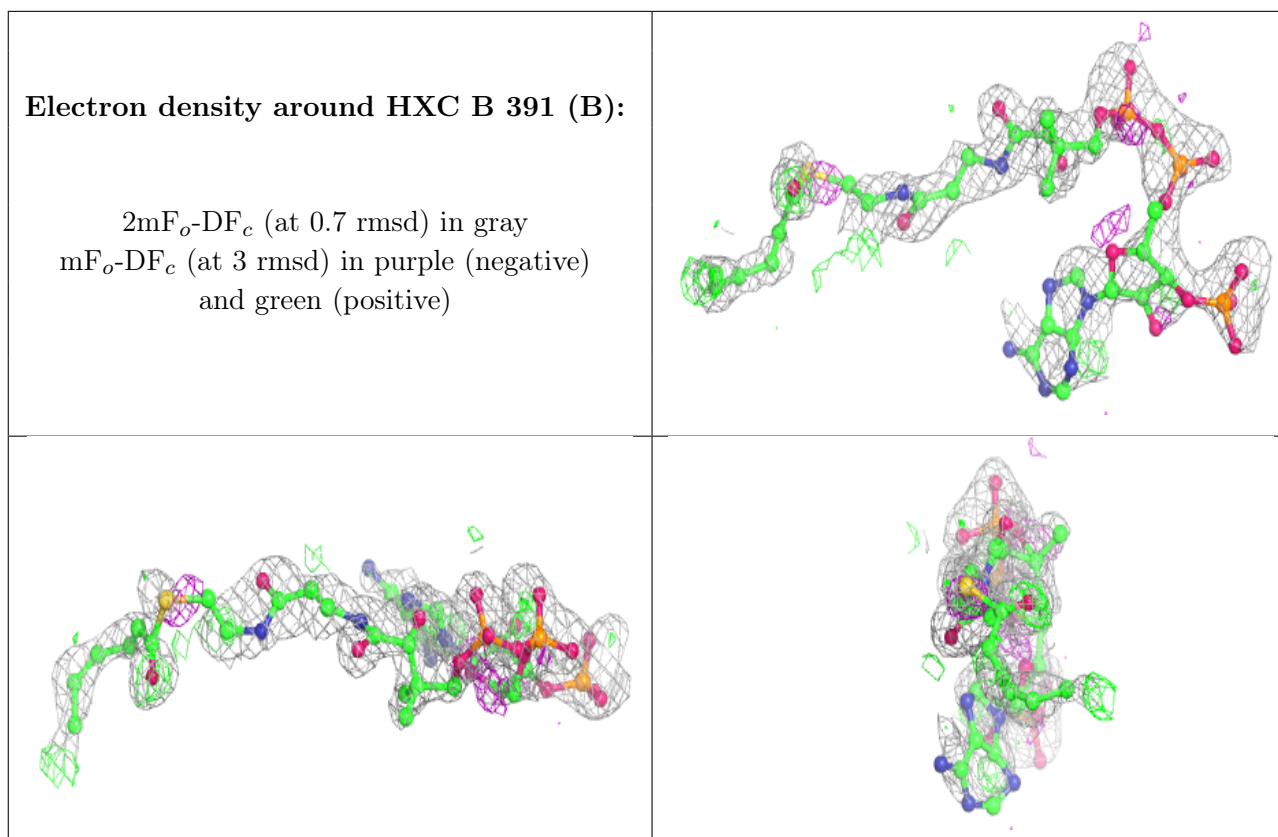
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.