



Full wwPDB X-ray Structure Validation Report

Aug 8, 2014 – 01:55 PM EDT

PDB ID : 4D0Z
Title : GalNAc-T2 crystal soaked with UDP-5SGalNAc, mEA2 and manganese (Higher resolution dataset)
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.
Deposited on : 2014-04-30
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

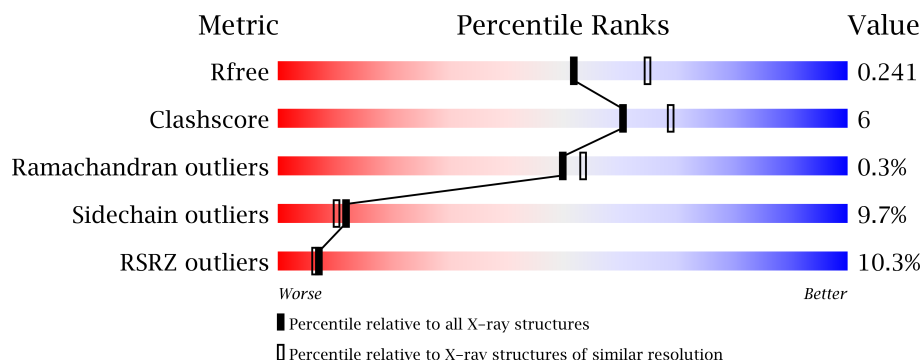
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	
1	C	571	
1	D	571	
1	E	571	
1	F	571	
2	X	6	
2	Y	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	A	1571	-	X
4	EDO	A	1572	-	X
4	EDO	A	1573	-	X
4	EDO	A	1576	-	X
4	EDO	A	1577	-	X
4	EDO	A	1579	-	X
4	EDO	A	1580	-	X
4	EDO	B	1573	-	X
4	EDO	B	1575	-	X
4	EDO	B	1576	-	X
4	EDO	B	1578	-	X
4	EDO	D	1576	-	X
4	EDO	D	1577	-	X
4	EDO	E	1570	-	X
4	EDO	E	1573	-	X
4	EDO	E	1576	-	X
4	EDO	E	1577	-	X
4	EDO	E	1578	-	X
4	EDO	E	1580	-	X
4	EDO	E	1581	-	X
5	BBK	B	1580	-	X
5	BBK	D	1572	-	X
5	BBK	E	1584	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24773 atoms, of which 0 are hydrogen and 0 are deuterium.

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 POLYPEPTIDE N-ACETYLGALACTOSAMINYLTRANSFERASE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	20	1	0
			3975	2502	722	727	24			
1	B	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	C	476	Total	C	N	O	S	20	0	0
			3826	2407	693	702	24			
1	D	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	E	495	Total	C	N	O	S	20	0	0
			3967	2497	719	727	24			
1	F	491	Total	C	N	O	S	20	0	0
			3926	2470	710	722	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
B	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
C	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
D	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
E	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471
F	516	ASP	ASN	ENGINEERED MUTATION	UNP Q10471

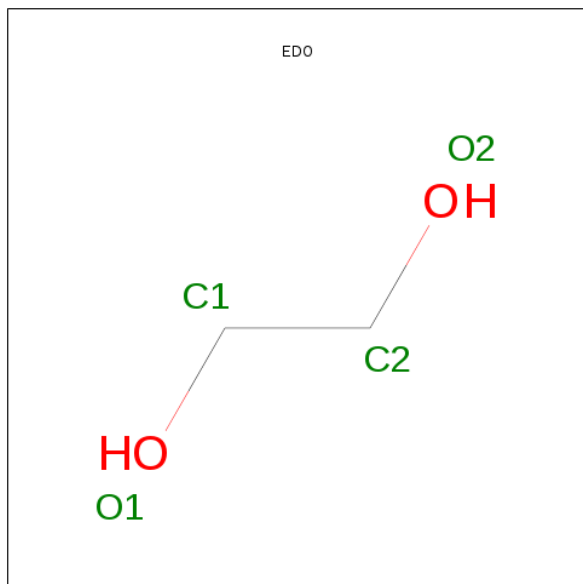
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			
2	Y	6	Total	C	N	O	S	0	0	1
			32	18	6	7	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

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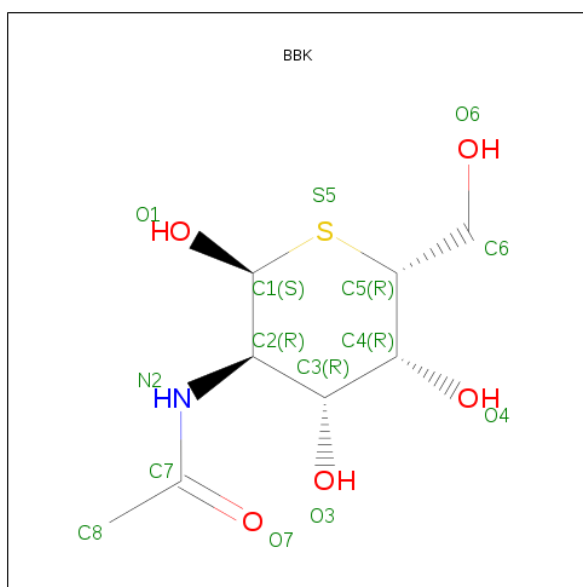
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-5-THIO-ALPHA-D-GALACTOPYRANOSE) (three-letter code: BBK) (formula: $C_8H_{15}NO_5S$).



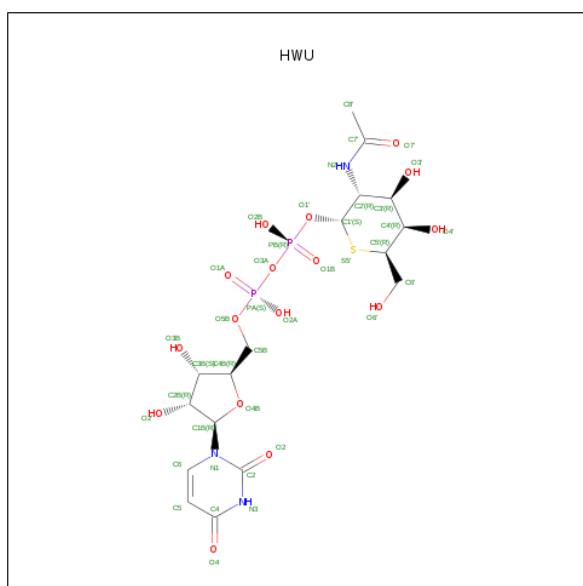
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	1	5	1		
5	E	1	Total	C	N	O	S	0	0
			15	8	1	5	1		

- Molecule 6 is (2R,3R,4R,5R,6R)-3-(ACETYLAMINO)-4,5-DIHYDROXY-6-(HYDROXYMETHYL)TETRAHYDRO-2H-THIOPYRAN-2-YL[(2R,3S,4R,5R)-5-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYLDIHYDROGEN DIPHOSPHATE (three-letter code: HWU) (formula: C₁₇H₂₇N₃O₁₆P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0
6	B	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0
6	C	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0
6	D	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0
6	E	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0
6	F	1	Total 39	C 17	N 3	O 16	P 2	S 1	0	0

- Molecule 7 is water.

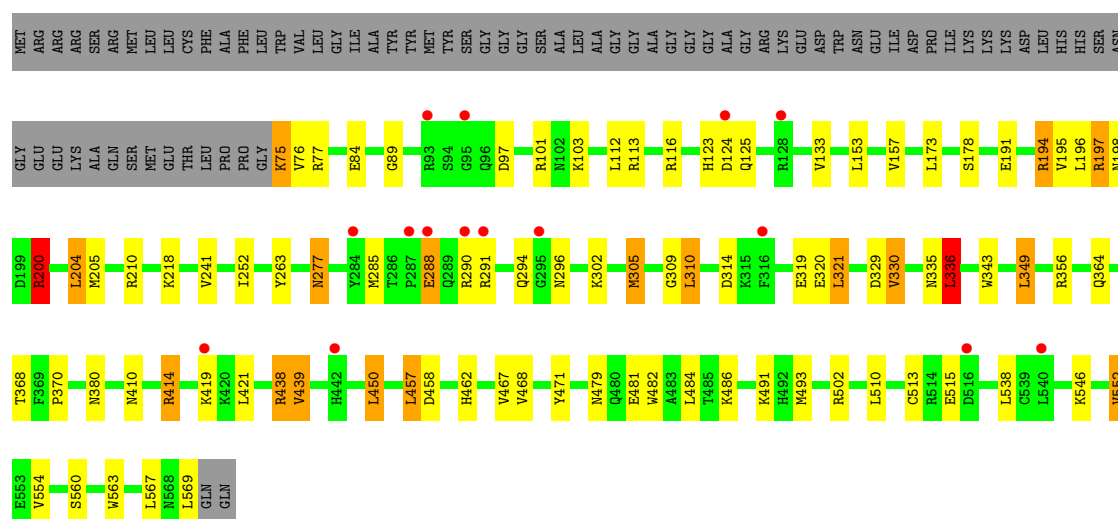
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	144	Total 144	O 144	0	0
7	B	125	Total 125	O 125	0	0
7	C	13	Total 13	O 13	0	0
7	D	122	Total 122	O 122	0	0
7	E	168	Total 168	O 168	0	0
7	F	61	Total 61	O 61	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

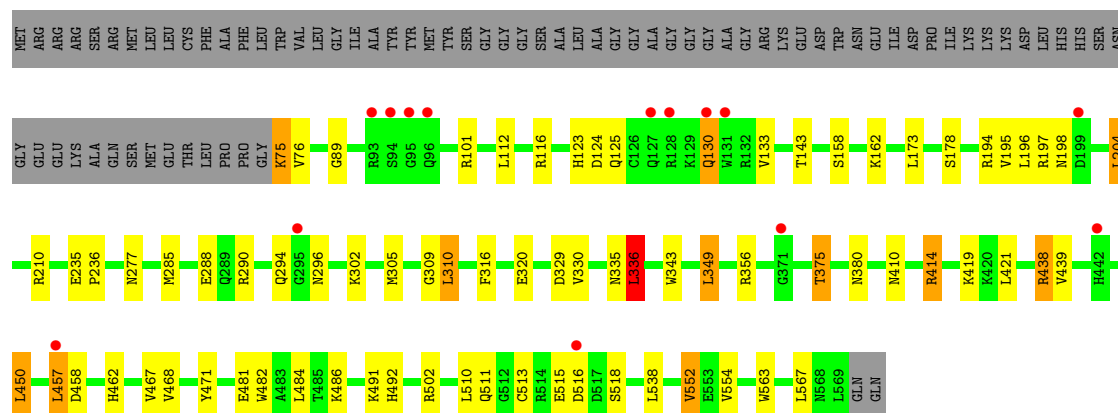
• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE2

Chain A: 



• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE2

Chain B: 



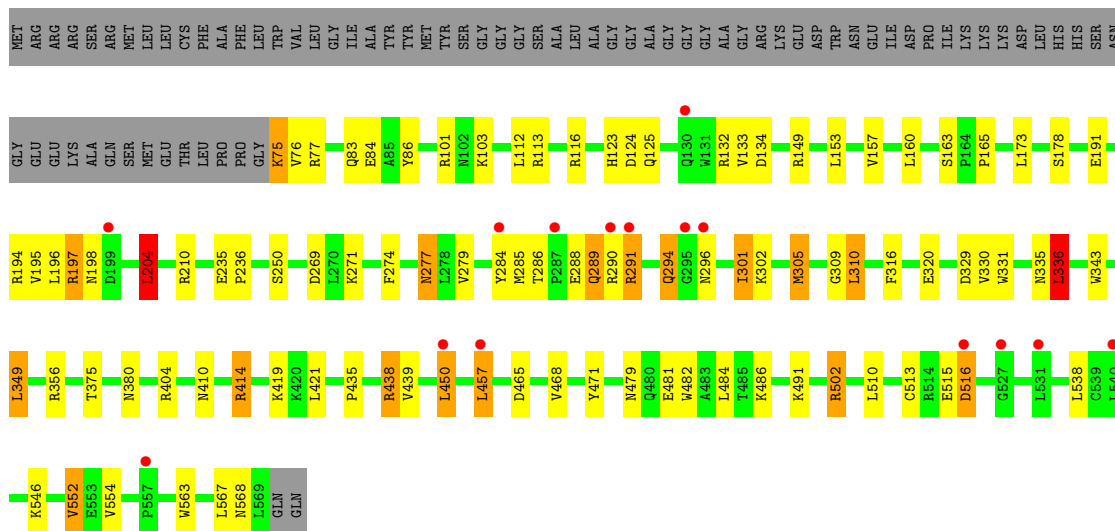
• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE2

Chain C: 



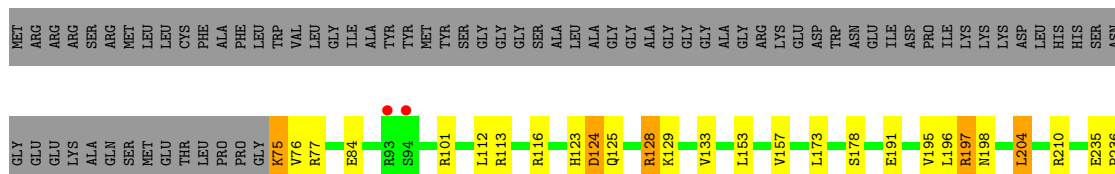
• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE2

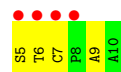
Chain D:



• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE2

Chain E:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.48Å 121.14Å 249.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.39 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (249.39-2.20) 99.8 (19.95-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.196 , 0.234 0.206 , 0.241	Depositor DCC
R_{free} test set	4936 reflections (2.85%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 178449 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24773	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HWU, BBK, EDO, MN

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	0.85	4/4070 (0.1%)	0.98	25/5503 (0.5%)
1	B	0.79	3/4059 (0.1%)	0.91	9/5489 (0.2%)
1	C	0.88	7/3912 (0.2%)	0.98	26/5287 (0.5%)
1	D	1.01	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	E	0.92	3/4059 (0.1%)	0.98	19/5489 (0.3%)
1	F	0.89	3/4015 (0.1%)	0.90	12/5427 (0.2%)
2	X	1.42	0/32	1.09	0/44
2	Y	1.82	1/32 (3.1%)	1.53	0/44
All	All	0.89	24/24238 (0.1%)	0.95	110/32772 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	F	0	1
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	75	LYS	CB-CG	-33.78	0.61	1.52
1	C	84	GLU	CB-CG	-26.41	1.01	1.52
1	D	486	LYS	CB-CG	-25.36	0.84	1.52
1	F	75	LYS	CB-CG	-25.00	0.85	1.52
1	E	84	GLU	CB-CG	-23.77	1.06	1.52
1	F	84	GLU	CB-CG	-23.05	1.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	486	LYS	CB-CG	-20.62	0.96	1.52
1	C	224	ASP	C-N	-20.14	0.87	1.34
1	A	84	GLU	CB-CG	-16.34	1.21	1.52
1	A	75	LYS	CB-CG	-14.91	1.12	1.52
1	C	225	SER	C-N	-14.91	0.99	1.34
1	E	75	LYS	CB-CG	-14.21	1.14	1.52
1	C	222	PHE	C-N	12.92	1.63	1.34
1	B	75	LYS	CB-CG	-12.78	1.18	1.52
1	A	486	LYS	CB-CG	-10.92	1.23	1.52
1	C	486	LYS	CB-CG	-10.47	1.24	1.52
1	B	515	GLU	CB-CG	-9.63	1.33	1.52
1	C	223	LEU	C-N	7.13	1.50	1.34
1	C	75	LYS	CB-CG	-6.90	1.33	1.52
2	Y	9	ALA	C-O	6.73	1.36	1.23
1	B	294	GLN	CB-CG	6.40	1.69	1.52
1	A	294	GLN	CB-CG	5.63	1.67	1.52
1	E	294	GLN	CB-CG	5.50	1.67	1.52
1	D	250	SER	CB-OG	-5.18	1.35	1.42

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	CA-CB-CG	21.27	160.19	113.40
1	D	194	ARG	NE-CZ-NH2	-17.68	111.46	120.30
1	E	75	LYS	CA-CB-CG	16.43	149.55	113.40
1	F	75	LYS	CA-CB-CG	15.46	147.41	113.40
1	D	75	LYS	CB-CG-CD	13.48	146.66	111.60
1	E	486	LYS	CB-CG-CD	-12.84	78.21	111.60
1	C	75	LYS	CA-CB-CG	12.77	141.48	113.40
1	B	486	LYS	CB-CG-CD	-11.69	81.22	111.60
1	F	84	GLU	CA-CB-CG	11.10	137.83	113.40
1	A	200	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	D	75	LYS	CA-CB-CG	10.92	137.41	113.40
1	C	225	SER	O-C-N	-10.49	105.92	122.70
1	D	194	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	E	84	GLU	CA-CB-CG	10.22	135.89	113.40
1	D	204	LEU	CA-CB-CG	9.38	136.88	115.30
1	C	225	SER	CA-C-N	9.35	137.77	117.20
1	B	486	LYS	CA-CB-CG	-9.22	93.12	113.40
1	C	567	LEU	CA-CB-CG	9.10	136.22	115.30
1	E	486	LYS	CA-CB-CG	-9.09	93.40	113.40
1	A	486	LYS	CB-CG-CD	-9.09	87.98	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	GLN	CB-CG-CD	8.58	133.90	111.60
1	A	84	GLU	CA-CB-CG	8.46	132.02	113.40
1	C	223	LEU	O-C-N	-8.39	109.28	122.70
1	B	204	LEU	CA-CB-CG	8.37	134.54	115.30
1	C	471	TYR	CA-CB-CG	8.19	128.96	113.40
1	C	84	GLU	CA-CB-CG	8.12	131.27	113.40
1	E	204	LEU	CA-CB-CG	8.07	133.86	115.30
1	D	414	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	294	GLN	CA-CB-CG	-7.93	95.96	113.40
1	C	225	SER	N-CA-C	-7.82	89.90	111.00
1	A	321	LEU	N-CA-C	-7.78	90.00	111.00
1	E	128	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	225	SER	C-N-CA	7.48	140.40	121.70
1	B	414	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	D	404	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	414	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	E	129	LYS	CD-CE-NZ	7.32	128.55	111.70
1	D	414	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	E	414	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	294	GLN	CB-CG-CD	6.98	129.75	111.60
1	E	532	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	113	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	527	GLY	N-CA-C	-6.88	95.89	113.10
1	A	197	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	414	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	414	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	567	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	200	ARG	CD-NE-CZ	6.52	132.73	123.60
1	F	294	GLN	CA-CB-CG	-6.50	99.10	113.40
1	C	439	VAL	CB-CA-C	6.48	123.71	111.40
1	B	414	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	E	294	GLN	CB-CG-CD	6.41	128.28	111.60
1	F	356	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	F	414	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	302	LYS	N-CA-C	6.33	128.09	111.00
1	C	223	LEU	C-N-CA	6.30	137.46	121.70
1	A	197	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[A]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	194[B]	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	356	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	194	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	314	ASP	CB-CG-OD2	-6.05	112.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	330	VAL	CA-CB-CG2	-6.01	101.89	110.90
1	A	486	LYS	CA-CB-CG	-5.99	100.22	113.40
1	E	336	LEU	CA-CB-CG	5.97	129.03	115.30
1	D	103	LYS	CD-CE-NZ	5.91	125.30	111.70
1	E	414	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	197	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	336	LEU	CA-CB-CG	5.85	128.75	115.30
1	F	336	LEU	CA-CB-CG	5.84	128.74	115.30
1	E	532	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	F	356	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	294	GLN	CA-CB-CG	-5.75	100.75	113.40
1	A	97	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	305	MET	CG-SD-CE	-5.68	91.11	100.20
1	F	567	LEU	CA-CB-CG	5.62	128.23	115.30
1	C	336	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	336	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	321	LEU	CA-C-N	5.57	127.33	116.20
1	E	356	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	414	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	D	404	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	75	LYS	CA-CB-CG	5.50	125.49	113.40
1	D	197	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	336	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	194[A]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	194[B]	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	77	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	362	ARG	CG-CD-NE	5.38	123.11	111.80
1	E	84	GLU	CB-CG-CD	5.38	128.74	114.20
1	C	97	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	197	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	197	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	486	LYS	CA-CB-CG	5.28	125.02	113.40
1	C	532	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	567	LEU	CA-CB-CG	5.25	127.38	115.30
1	E	438	ARG	CB-CG-CD	5.25	125.25	111.60
1	E	305	MET	CG-SD-CE	-5.24	91.81	100.20
1	C	477	GLY	N-CA-C	5.23	126.18	113.10
1	D	305	MET	CG-SD-CE	-5.22	91.85	100.20
1	C	218	LYS	CB-CA-C	-5.18	100.03	110.40
1	B	356	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	113	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	356	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	569	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C	194	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	218	LYS	CB-CA-C	-5.07	100.27	110.40
1	D	113	ARG	N-CA-CB	-5.03	101.54	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	GLY	Peptide
1	B	89	GLY	Peptide
1	C	223	LEU	Mainchain
1	F	89	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3975	0	3903	53	0
1	B	3967	0	3890	28	0
1	C	3826	0	3748	78	0
1	D	3967	0	3890	53	0
1	E	3967	0	3890	47	0
1	F	3926	0	3849	32	0
2	X	32	0	28	2	0
2	Y	32	0	28	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	40	0	60	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	48	6	0
4	D	20	0	30	5	0
4	E	56	0	84	15	0
5	A	15	0	0	3	0
5	B	15	0	0	2	0
5	D	15	0	0	2	0
5	E	15	0	0	3	0
6	A	39	0	0	0	0
6	B	39	0	0	1	0
6	C	39	0	0	6	0
6	D	39	0	0	0	0
6	E	39	0	0	1	0
6	F	39	0	0	2	0
7	A	144	0	0	0	0
7	B	125	0	0	3	0
7	C	13	0	0	6	0
7	D	122	0	0	3	0
7	E	168	0	0	3	0
7	F	61	0	0	0	0
All	All	24773	0	23448	281	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (281) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:203:GLY:HA3	1:C:330:VAL:CG2	1.71	1.19
1:C:203:GLY:CA	1:C:330:VAL:CG2	2.26	1.13
1:A:291:ARG:CZ	1:D:435:PRO:HB2	1.79	1.11
1:C:203:GLY:HA3	1:C:330:VAL:HG22	1.20	1.10
1:C:330:VAL:HG12	1:C:331:TRP:HB3	1.32	1.08
1:C:203:GLY:HA2	1:C:330:VAL:HG21	1.33	1.08
1:C:203:GLY:CA	1:C:330:VAL:HG22	1.88	1.01
1:C:203:GLY:CA	1:C:330:VAL:HG21	1.92	0.98
1:D:271:LYS:HG2	1:D:301:ILE:HD11	1.46	0.96
1:C:330:VAL:HG11	6:C:1569:HWU:C5	1.99	0.92
1:C:145:HIS:CD2	1:C:201:ARG:HH21	1.91	0.89
1:A:291:ARG:CZ	1:D:435:PRO:CB	2.54	0.85
1:C:203:GLY:HA2	1:C:330:VAL:CG2	2.03	0.80
1:F:134:ASP:O	1:F:134:ASP:OD1	2.00	0.80
1:F:438:ARG:HG2	1:F:481:GLU:OE2	1.82	0.79
1:F:524:GLN:HG2	1:F:528:ASN:HA	1.63	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:474:HIS:HD2	1:F:476:ALA:H	1.30	0.78
1:C:114:MET:HA	7:C:2004:HOH:O	1.84	0.78
1:D:123:HIS:HD2	1:D:125:GLN:H	1.32	0.77
1:D:438:ARG:HG2	1:D:481:GLU:OE2	1.83	0.77
1:C:474:HIS:HD2	1:C:476:ALA:H	1.30	0.77
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.20	0.77
1:A:438:ARG:HG2	1:A:481:GLU:OE2	1.86	0.76
1:A:439:VAL:H	1:D:291:ARG:NH2	1.84	0.75
1:F:123:HIS:HD2	1:F:125:GLN:H	1.33	0.74
1:B:438:ARG:HG2	1:B:481:GLU:OE2	1.88	0.74
1:D:165:PRO:HA	4:D:1576:EDO:H22	1.69	0.74
1:C:123:HIS:HD2	1:C:125:GLN:H	1.36	0.74
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.22	0.73
1:E:123:HIS:HD2	1:E:125:GLN:H	1.33	0.72
1:D:516:ASP:OD1	1:D:516:ASP:N	2.22	0.72
1:A:123:HIS:HD2	1:A:125:GLN:H	1.36	0.72
1:B:123:HIS:HD2	1:B:125:GLN:H	1.37	0.72
1:A:291:ARG:NH1	1:D:435:PRO:HB2	2.05	0.71
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.25	0.71
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.25	0.70
1:D:277:ASN:ND2	1:D:279:VAL:HG12	2.06	0.70
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.26	0.70
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.25	0.70
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.57	0.69
1:E:438:ARG:HG2	1:E:481:GLU:OE2	1.93	0.69
1:C:277:ASN:ND2	1:C:279:VAL:HG12	2.08	0.69
4:B:1573:EDO:H12	7:B:2011:HOH:O	1.92	0.68
1:C:439:VAL:C	1:C:440:PRO:O	2.30	0.68
1:F:316:PHE:CE2	1:F:320:GLU:OE2	2.47	0.68
1:A:320:GLU:C	1:A:321:LEU:O	2.28	0.67
1:C:145:HIS:CE1	1:C:201:ARG:HE	2.12	0.67
1:C:439:VAL:O	1:C:440:PRO:O	2.12	0.66
1:D:286:THR:OG1	1:D:289:GLN:HG2	1.95	0.66
1:D:329:ASP:H	1:D:380:ASN:HD21	1.41	0.66
1:E:458:ASP:OD1	5:E:1584:BBK:O3	2.14	0.66
1:C:204:LEU:H	1:C:330:VAL:HG13	1.62	0.65
1:C:329:ASP:H	1:C:380:ASN:HD21	1.45	0.65
1:C:225:SER:O	1:C:226:HIS:CG	2.51	0.64
1:C:439:VAL:O	1:C:440:PRO:C	2.37	0.63
1:B:458:ASP:OD1	5:B:1580:BBK:O3	2.17	0.62
1:C:205:MET:HE3	1:C:328:MET:O	2.00	0.62
1:F:368:THR:HG22	1:F:370:PRO:HD3	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:TYR:H	4:A:1580:EDO:H21	1.65	0.62
6:C:1569:HWU:O3A	6:C:1569:HWU:O6'	2.18	0.62
1:A:194[B]:ARG:HG2	1:A:194[B]:ARG:HH11	1.65	0.62
1:F:329:ASP:H	1:F:380:ASN:HD21	1.48	0.62
1:A:368:THR:HG22	1:A:370:PRO:HD3	1.82	0.62
1:B:316:PHE:CE2	1:B:320:GLU:OE2	2.53	0.62
1:B:162:LYS:HE3	4:B:1573:EDO:O2	1.99	0.61
1:F:460:LEU:CD2	1:F:471:TYR:CE2	2.84	0.61
1:E:329:ASP:H	1:E:380:ASN:HD21	1.48	0.61
1:E:368:THR:HG22	1:E:370:PRO:HD3	1.83	0.60
1:E:479:ASN:HD22	5:E:1584:BBK:C3	2.14	0.60
1:B:329:ASP:H	1:B:380:ASN:HD21	1.48	0.60
1:C:316:PHE:CE2	1:C:320:GLU:OE2	2.55	0.60
1:D:160:LEU:HA	4:D:1576:EDO:H12	1.83	0.60
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.49	0.60
1:B:305:MET:HE1	1:B:336:LEU:CD2	2.32	0.60
1:D:305:MET:HE1	1:D:336:LEU:CD2	2.32	0.59
1:A:329:ASP:H	1:A:380:ASN:HD21	1.50	0.59
1:C:145:HIS:CD2	1:C:201:ARG:NH2	2.67	0.59
1:D:277:ASN:HD21	1:D:279:VAL:HG12	1.66	0.59
1:D:414:ARG:HD3	7:D:2082:HOH:O	2.01	0.59
1:D:316:PHE:CE2	1:D:320:GLU:OE2	2.56	0.58
1:E:278:LEU:O	4:E:1572:EDO:C1	2.51	0.58
1:C:176:ASP:OD2	1:C:203:GLY:N	2.34	0.58
7:C:2001:HOH:O	1:E:113:ARG:NH2	2.34	0.58
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.52	0.58
1:D:305:MET:HE1	1:D:336:LEU:HD23	1.85	0.58
6:B:1571:HWU:C1'	2:X:6:THR:OG1	2.52	0.58
1:A:560:SER:HB3	4:A:1579:EDO:H12	1.86	0.57
1:C:277:ASN:HD21	1:C:279:VAL:HG12	1.68	0.57
1:F:460:LEU:HD22	1:F:471:TYR:CE2	2.39	0.57
1:C:205:MET:HE2	1:C:205:MET:H	1.68	0.57
1:B:305:MET:HE1	1:B:336:LEU:HD23	1.86	0.57
1:C:77:ARG:CG	1:C:80:ASP:OD2	2.53	0.57
1:C:517:ASP:O	1:C:521:LYS:HE2	2.04	0.56
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.54	0.56
1:A:305:MET:HE1	1:A:336:LEU:CD2	2.36	0.56
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.54	0.56
1:E:333:GLY:N	4:E:1572:EDO:H21	2.21	0.56
1:E:438:ARG:CG	1:E:481:GLU:OE2	2.54	0.56
1:C:305:MET:HE1	1:C:336:LEU:CD2	2.36	0.55
1:C:305:MET:HE1	1:C:336:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:271:LYS:CG	1:D:301:ILE:HD11	2.29	0.55
1:D:479:ASN:HB2	5:D:1572:BBK:C4	2.36	0.55
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.54	0.55
6:E:1585:HWU:O1B	2:Y:5:SER:N	2.38	0.55
1:E:333:GLY:H	4:E:1572:EDO:H21	1.72	0.55
1:A:305:MET:HE1	1:A:336:LEU:HD23	1.90	0.54
1:E:414:ARG:HD3	7:E:2102:HOH:O	2.05	0.54
1:C:471:TYR:CD1	1:F:472:GLU:OE1	2.60	0.54
1:E:492:HIS:HA	4:E:1582:EDO:H11	1.90	0.53
1:C:331:TRP:HE1	1:C:365:HIS:CE1	2.26	0.53
1:B:516:ASP:OD1	1:C:117:ALA:HB3	2.09	0.53
1:C:471:TYR:OH	1:F:473:CYS:O	2.26	0.53
1:B:492:HIS:HA	4:B:1577:EDO:H21	1.91	0.52
1:B:462:HIS:HD2	1:B:467:VAL:O	1.92	0.52
1:E:124:ASP:HB3	1:E:128:ARG:NH2	2.25	0.52
1:C:270:LEU:HD21	1:F:463:PHE:CE1	2.45	0.52
1:A:364:GLN:HE21	4:A:1572:EDO:C1	2.22	0.52
1:D:163:SER:O	4:D:1576:EDO:O1	2.28	0.52
1:C:77:ARG:H	1:C:77:ARG:CD	2.22	0.52
1:E:462:HIS:HD2	1:E:467:VAL:O	1.93	0.52
1:C:329:ASP:O	1:C:330:VAL:C	2.46	0.51
1:E:364:GLN:HE21	4:E:1573:EDO:H22	1.75	0.51
1:F:127:GLN:C	1:F:128:ARG:HD3	2.31	0.51
1:D:286:THR:OG1	1:D:289:GLN:CG	2.59	0.51
6:C:1569:HWU:PA	6:C:1569:HWU:O6'	2.68	0.51
1:C:471:TYR:CE2	1:F:472:GLU:HB3	2.46	0.51
1:E:333:GLY:HA2	4:E:1572:EDO:C2	2.40	0.51
1:D:414:ARG:CD	7:D:2082:HOH:O	2.57	0.50
1:A:291:ARG:NH2	1:D:435:PRO:CB	2.73	0.50
1:E:500:VAL:O	4:E:1580:EDO:H22	2.12	0.50
1:A:493:MET:HB3	1:D:269:ASP:OD2	2.12	0.49
1:B:158:SER:HB3	4:B:1573:EDO:H11	1.94	0.49
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.59	0.49
1:C:515:GLU:O	1:C:521:LYS:NZ	2.36	0.49
1:E:333:GLY:H	4:E:1572:EDO:C2	2.25	0.49
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.47	0.49
1:A:491:LYS:HE2	1:A:513:CYS:SG	2.52	0.49
1:B:491:LYS:HE2	1:B:513:CYS:SG	2.52	0.49
1:A:479:ASN:HD22	5:A:1581:BBK:C3	2.25	0.48
1:C:462:HIS:HD2	1:C:467:VAL:O	1.95	0.48
1:E:293:ARG:HD2	4:E:1570:EDO:H22	1.95	0.48
1:C:412:GLN:HB3	7:C:2013:HOH:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:MET:HE3	1:A:305:MET:HB2	1.61	0.48
1:A:305:MET:CE	1:A:336:LEU:HD23	2.43	0.48
1:D:305:MET:CE	1:D:336:LEU:HD23	2.44	0.48
1:C:305:MET:CE	1:C:336:LEU:HD23	2.43	0.48
1:D:235:GLU:N	1:D:236:PRO:CD	2.77	0.48
1:A:364:GLN:HE21	4:A:1572:EDO:H12	1.79	0.48
1:C:412:GLN:CB	7:C:2013:HOH:O	2.62	0.48
1:A:200:ARG:NH1	1:A:200:ARG:HG2	2.26	0.47
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.49	0.47
1:A:462:HIS:HD2	1:A:467:VAL:O	1.96	0.47
1:F:491:LYS:HE2	1:F:513:CYS:SG	2.54	0.47
1:F:538:LEU:HB3	1:F:552:VAL:HG22	1.96	0.47
6:C:1569:HWU:O3A	6:C:1569:HWU:C5'	2.62	0.47
1:E:239:GLU:OE2	7:E:2030:HOH:O	2.20	0.47
1:B:343:TRP:CD1	1:B:349:LEU:HD22	2.49	0.47
1:C:491:LYS:HE2	1:C:513:CYS:SG	2.54	0.47
1:C:204:LEU:HD12	1:C:205:MET:N	2.29	0.47
1:F:204:LEU:HD12	1:F:205:MET:N	2.29	0.47
1:C:331:TRP:CZ2	1:C:365:HIS:CG	3.02	0.47
1:E:305:MET:HB2	1:E:305:MET:HE3	1.60	0.47
1:E:278:LEU:O	4:E:1572:EDO:H12	2.14	0.47
1:B:305:MET:HB2	1:B:305:MET:HE3	1.69	0.47
1:E:305:MET:CE	1:E:336:LEU:HD23	2.45	0.47
1:C:77:ARG:NE	1:C:80:ASP:OD2	2.46	0.47
1:A:288:GLU:HA	1:A:291:ARG:NH1	2.30	0.47
1:A:277:ASN:O	4:A:1575:EDO:O1	2.20	0.47
1:F:343:TRP:CD1	1:F:349:LEU:HD22	2.50	0.47
1:B:178:SER:O	1:B:197:ARG:NH2	2.42	0.47
1:E:333:GLY:HA2	4:E:1572:EDO:H22	1.97	0.47
1:E:491:LYS:HE2	1:E:513:CYS:SG	2.54	0.47
1:C:538:LEU:HB3	1:C:552:VAL:HG22	1.96	0.46
1:E:305:MET:HE1	1:E:336:LEU:CD2	2.45	0.46
1:A:538:LEU:HB3	1:A:552:VAL:HG22	1.98	0.46
1:D:165:PRO:CA	4:D:1576:EDO:H22	2.44	0.46
1:C:155:THR:HG1	1:C:226:HIS:N	2.14	0.46
1:D:491:LYS:HE2	1:D:513:CYS:SG	2.55	0.46
1:A:439:VAL:H	1:D:291:ARG:HH21	1.59	0.46
1:A:291:ARG:NH2	1:D:435:PRO:HB2	2.27	0.46
1:F:178:SER:O	1:F:197:ARG:NH2	2.43	0.46
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.51	0.46
1:E:178:SER:O	1:E:197:ARG:NH2	2.42	0.46
1:F:309:GLY:C	1:F:310:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:GLU:O	1:A:191:GLU:HG3	2.16	0.45
1:A:309:GLY:C	1:A:310:LEU:HD23	2.36	0.45
1:A:319:GLU:O	1:A:321:LEU:O	2.34	0.45
1:C:205:MET:CE	1:C:328:MET:O	2.64	0.45
1:C:305:MET:HE3	1:C:305:MET:HB2	1.64	0.45
1:D:274:PHE:CD2	1:D:305:MET:HE1	2.51	0.45
1:E:493:MET:H	4:E:1582:EDO:H22	1.80	0.45
1:C:178:SER:O	1:C:197:ARG:NH2	2.40	0.45
1:E:414:ARG:CD	7:E:2102:HOH:O	2.63	0.45
1:C:204:LEU:HG	1:C:330:VAL:HG13	1.97	0.45
1:D:465:ASP:OD1	4:D:1573:EDO:H11	2.17	0.44
1:E:479:ASN:HB2	5:E:1584:BBK:C4	2.47	0.44
1:C:189:LYS:NZ	7:C:2008:HOH:O	2.49	0.44
1:E:191:GLU:O	1:E:191:GLU:HG3	2.17	0.44
1:E:309:GLY:C	1:E:310:LEU:HD23	2.38	0.44
1:F:235:GLU:N	1:F:236:PRO:CD	2.80	0.44
1:C:303:THR:HA	1:C:304:PRO:HD3	1.96	0.44
1:D:285:MET:O	1:D:290:ARG:NH1	2.51	0.44
1:A:103:LYS:HD2	4:A:1572:EDO:H12	1.98	0.44
1:A:178:SER:O	1:A:197:ARG:NH2	2.42	0.44
1:A:204:LEU:HD12	1:A:205:MET:N	2.32	0.44
1:B:518:SER:HB3	1:C:161:LYS:NZ	2.32	0.44
1:C:106:GLN:HB2	7:C:2003:HOH:O	2.17	0.44
1:A:263:TYR:N	4:A:1580:EDO:H21	2.31	0.44
1:A:252:ILE:HG23	4:A:1578:EDO:H11	2.00	0.44
1:B:235:GLU:N	1:B:236:PRO:CD	2.81	0.44
1:B:305:MET:CE	1:B:336:LEU:HD23	2.47	0.44
1:A:479:ASN:HB2	5:A:1581:BBK:C4	2.48	0.44
1:E:335:ASN:HD21	4:E:1572:EDO:C2	2.31	0.44
1:D:132:ARG:HB2	1:D:134:ASP:OD1	2.18	0.43
1:D:538:LEU:HB3	1:D:552:VAL:HG22	1.98	0.43
1:B:538:LEU:HB3	1:B:552:VAL:HG22	2.00	0.43
1:D:305:MET:HE3	1:D:305:MET:HB2	1.62	0.43
1:C:77:ARG:H	1:C:77:ARG:HD3	1.81	0.43
1:C:176:ASP:OD1	1:C:202:GLU:N	2.38	0.43
1:C:200:ARG:O	1:C:202:GLU:HG2	2.19	0.43
1:C:205:MET:HE3	1:C:205:MET:HB2	1.86	0.43
1:D:153:LEU:O	1:D:157:VAL:HG13	2.19	0.43
1:E:335:ASN:N	1:E:335:ASN:HD22	2.16	0.43
1:C:191:GLU:O	1:C:191:GLU:HG3	2.19	0.43
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.53	0.43
1:E:235:GLU:N	1:E:236:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:375:THR:HG23	7:B:2079:HOH:O	2.18	0.43
1:C:205:MET:CE	1:C:205:MET:H	2.32	0.42
1:C:285:MET:O	1:C:290:ARG:NH1	2.52	0.42
1:D:178:SER:O	1:D:197:ARG:NH2	2.40	0.42
1:F:191:GLU:O	1:F:191:GLU:HG3	2.18	0.42
4:B:1573:EDO:C1	7:B:2011:HOH:O	2.59	0.42
1:C:309:GLY:C	1:C:310:LEU:HD23	2.39	0.42
1:D:191:GLU:HG3	1:D:191:GLU:O	2.20	0.42
1:D:204:LEU:HD13	1:D:331:TRP:HA	2.02	0.42
1:A:291:ARG:NE	1:D:435:PRO:CB	2.82	0.42
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.01	0.42
1:A:364:GLN:NE2	4:A:1572:EDO:H12	2.34	0.42
1:E:153:LEU:O	1:E:157:VAL:HG13	2.19	0.42
1:E:285:MET:O	1:E:290:ARG:NH1	2.52	0.42
1:E:377:PHE:CE2	4:E:1579:EDO:H21	2.54	0.42
1:F:309:GLY:CA	6:F:1571:HWU:O3'	2.67	0.42
1:B:309:GLY:C	1:B:310:LEU:HD23	2.39	0.42
1:A:439:VAL:HG13	1:D:291:ARG:NH2	2.35	0.42
1:C:331:TRP:NE1	1:C:365:HIS:CE1	2.88	0.42
1:E:305:MET:CE	1:E:336:LEU:CD2	2.98	0.42
5:B:1580:BBK:C8	1:E:474:HIS:HB2	2.50	0.42
1:F:334:GLU:OE2	6:F:1571:HWU:O4'	2.38	0.42
1:A:153:LEU:O	1:A:157:VAL:HG13	2.20	0.42
1:D:86:TYR:CE2	1:D:149:ARG:HB3	2.55	0.42
1:A:285:MET:O	1:A:290:ARG:NH1	2.53	0.42
1:A:458:ASP:OD1	5:A:1581:BBK:O3	2.37	0.42
1:C:224:ASP:OD2	6:C:1569:HWU:O2B	2.37	0.42
1:D:502:ARG:HD2	7:D:2111:HOH:O	2.18	0.42
1:E:305:MET:HE1	1:E:336:LEU:HD23	2.00	0.42
1:D:450:LEU:HD13	1:D:563:TRP:CE3	2.55	0.42
1:F:285:MET:O	1:F:290:ARG:NH1	2.53	0.42
2:X:7:CYS:HA	2:X:8:PRO:HD3	1.89	0.42
1:C:291:ARG:NE	1:F:435:PRO:HB2	2.34	0.41
1:C:330:VAL:HG11	6:C:1569:HWU:C4	2.48	0.41
1:A:305:MET:CE	1:A:336:LEU:CD2	2.97	0.41
1:B:130:GLN:HB3	1:B:130:GLN:HE21	1.67	0.41
1:B:285:MET:O	1:B:290:ARG:NH1	2.53	0.41
1:F:153:LEU:O	1:F:157:VAL:HG13	2.19	0.41
1:A:439:VAL:H	1:D:291:ARG:HH22	1.64	0.41
1:C:225:SER:O	1:C:226:HIS:ND1	2.53	0.41
1:C:305:MET:CE	1:C:336:LEU:CD2	2.98	0.41
1:F:514:ARG:C	1:F:516:ASP:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:450:LEU:HD13	1:B:563:TRP:CE3	2.55	0.41
1:C:204:LEU:N	1:C:330:VAL:HG13	2.31	0.41
1:D:479:ASN:HD22	5:D:1572:BBK:C3	2.34	0.41
1:A:457:LEU:HD13	1:A:482:TRP:CZ2	2.56	0.41
1:D:309:GLY:C	1:D:310:LEU:HD23	2.41	0.41
1:E:377:PHE:CE2	4:E:1579:EDO:C2	3.04	0.41
1:B:511:GLN:NE2	4:B:1572:EDO:H21	2.36	0.41
1:F:460:LEU:HD23	1:F:471:TYR:CE2	2.56	0.41
1:A:450:LEU:HD13	1:A:563:TRP:CE3	2.56	0.41
1:C:515:GLU:O	1:C:517:ASP:N	2.54	0.41
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.17	0.40
1:D:83:GLN:HG2	1:D:84:GLU:N	2.35	0.40
1:C:271:LYS:HB2	1:C:271:LYS:HE3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/571 (86%)	479 (97%)	14 (3%)	1 (0%)	56	62
1	B	493/571 (86%)	476 (97%)	16 (3%)	1 (0%)	56	62
1	C	470/571 (82%)	451 (96%)	16 (3%)	3 (1%)	33	32
1	D	493/571 (86%)	478 (97%)	14 (3%)	1 (0%)	56	62
1	E	493/571 (86%)	479 (97%)	13 (3%)	1 (0%)	56	62
1	F	487/571 (85%)	473 (97%)	13 (3%)	1 (0%)	56	62
2	X	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	Y	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	2938/3438 (86%)	2842 (97%)	88 (3%)	8 (0%)	50	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	VAL
1	C	440	PRO
1	B	330	VAL
1	C	332	GLY
1	C	516	ASP
1	D	330	VAL
1	F	330	VAL
1	E	330	VAL

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	429/485 (88%)	388 (90%)	41 (10%)	12	11
1	B	428/485 (88%)	390 (91%)	38 (9%)	14	13
1	C	414/485 (85%)	371 (90%)	43 (10%)	10	9
1	D	428/485 (88%)	385 (90%)	43 (10%)	11	10
1	E	428/485 (88%)	389 (91%)	39 (9%)	14	13
1	F	424/485 (87%)	382 (90%)	42 (10%)	11	10
2	X	4/4 (100%)	3 (75%)	1 (25%)	1	0
2	Y	4/4 (100%)	2 (50%)	2 (50%)	0	0
All	All	2559/2918 (88%)	2310 (90%)	249 (10%)	12	10

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	76	VAL
1	A	77	ARG
1	A	101	ARG
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	173	LEU
1	A	195	VAL

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Mol	Chain	Res	Type
1	A	196	LEU
1	A	200	ARG
1	A	204	LEU
1	A	241	VAL
1	A	277	ASN
1	A	288	GLU
1	A	296	ASN
1	A	302	LYS
1	A	310	LEU
1	A	330	VAL
1	A	335	ASN
1	A	336	LEU
1	A	349	LEU
1	A	410	ASN
1	A	414	ARG
1	A	419	LYS
1	A	421	LEU
1	A	438	ARG
1	A	439	VAL
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	471	TYR
1	A	484	LEU
1	A	502	ARG
1	A	510	LEU
1	A	515	GLU
1	A	546	LYS
1	A	552	VAL
1	A	554	VAL
1	A	567	LEU
1	B	75	LYS
1	B	76	VAL
1	B	101	ARG
1	B	112	LEU
1	B	116	ARG
1	B	124	ASP
1	B	130	GLN
1	B	133	VAL
1	B	143	THR
1	B	173	LEU
1	B	195	VAL

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Mol	Chain	Res	Type
1	B	196	LEU
1	B	204	LEU
1	B	277	ASN
1	B	288	GLU
1	B	296	ASN
1	B	302	LYS
1	B	310	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	375	THR
1	B	410	ASN
1	B	414	ARG
1	B	419	LYS
1	B	421	LEU
1	B	438	ARG
1	B	439	VAL
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	471	TYR
1	B	484	LEU
1	B	502	ARG
1	B	510	LEU
1	B	552	VAL
1	B	554	VAL
1	B	567	LEU
1	C	75	LYS
1	C	76	VAL
1	C	77	ARG
1	C	101	ARG
1	C	112	LEU
1	C	113	ARG
1	C	116	ARG
1	C	124	ASP
1	C	133	VAL
1	C	173	LEU
1	C	195	VAL
1	C	196	LEU
1	C	201	ARG
1	C	204	LEU
1	C	205	MET

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Mol	Chain	Res	Type
1	C	277	ASN
1	C	288	GLU
1	C	294	GLN
1	C	296	ASN
1	C	302	LYS
1	C	310	LEU
1	C	330	VAL
1	C	335	ASN
1	C	336	LEU
1	C	349	LEU
1	C	410	ASN
1	C	419	LYS
1	C	421	LEU
1	C	438	ARG
1	C	439	VAL
1	C	450	LEU
1	C	457	LEU
1	C	468	VAL
1	C	471	TYR
1	C	484	LEU
1	C	500	VAL
1	C	502	ARG
1	C	510	LEU
1	C	515	GLU
1	C	516	ASP
1	C	546	LYS
1	C	552	VAL
1	C	554	VAL
1	D	75	LYS
1	D	76	VAL
1	D	101	ARG
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	173	LEU
1	D	195	VAL
1	D	196	LEU
1	D	204	LEU
1	D	277	ASN
1	D	284	TYR
1	D	288	GLU

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Mol	Chain	Res	Type
1	D	289	GLN
1	D	291	ARG
1	D	294	GLN
1	D	296	ASN
1	D	301	ILE
1	D	302	LYS
1	D	310	LEU
1	D	335	ASN
1	D	336	LEU
1	D	349	LEU
1	D	375	THR
1	D	410	ASN
1	D	419	LYS
1	D	421	LEU
1	D	438	ARG
1	D	439	VAL
1	D	450	LEU
1	D	457	LEU
1	D	468	VAL
1	D	471	TYR
1	D	484	LEU
1	D	502	ARG
1	D	510	LEU
1	D	515	GLU
1	D	516	ASP
1	D	546	LYS
1	D	552	VAL
1	D	554	VAL
1	D	568	ASN
1	E	75	LYS
1	E	76	VAL
1	E	77	ARG
1	E	101	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	133	VAL
1	E	173	LEU
1	E	195	VAL
1	E	196	LEU
1	E	204	LEU
1	E	277	ASN

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Mol	Chain	Res	Type
1	E	288	GLU
1	E	294	GLN
1	E	296	ASN
1	E	302	LYS
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	375	THR
1	E	410	ASN
1	E	419	LYS
1	E	421	LEU
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	471	TYR
1	E	484	LEU
1	E	502	ARG
1	E	510	LEU
1	E	515	GLU
1	E	546	LYS
1	E	552	VAL
1	E	554	VAL
1	E	567	LEU
1	F	75	LYS
1	F	76	VAL
1	F	101	ARG
1	F	112	LEU
1	F	116	ARG
1	F	124	ASP
1	F	128	ARG
1	F	134	ASP
1	F	173	LEU
1	F	195	VAL
1	F	196	LEU
1	F	204	LEU
1	F	277	ASN
1	F	288	GLU
1	F	294	GLN
1	F	296	ASN

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Mol	Chain	Res	Type
1	F	302	LYS
1	F	310	LEU
1	F	335	ASN
1	F	336	LEU
1	F	349	LEU
1	F	375	THR
1	F	410	ASN
1	F	414	ARG
1	F	419	LYS
1	F	421	LEU
1	F	438	ARG
1	F	439	VAL
1	F	442	HIS
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	471	TYR
1	F	484	LEU
1	F	500	VAL
1	F	502	ARG
1	F	510	LEU
1	F	515	GLU
1	F	516	ASP
1	F	546	LYS
1	F	552	VAL
1	F	554	VAL
2	X	5	SER
2	Y	6	THR
2	Y	7	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	123	HIS
1	A	127	GLN
1	A	198	ASN
1	A	277	ASN
1	A	296	ASN
1	A	335	ASN
1	A	344	GLN
1	A	364	GLN

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Mol	Chain	Res	Type
1	A	365	HIS
1	A	380	ASN
1	A	410	ASN
1	A	432	ASN
1	A	452	GLN
1	A	462	HIS
1	A	479	ASN
1	A	537	ASN
1	B	106	GLN
1	B	123	HIS
1	B	127	GLN
1	B	130	GLN
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	365	HIS
1	B	380	ASN
1	B	410	ASN
1	B	451	GLN
1	B	452	GLN
1	B	462	HIS
1	B	537	ASN
1	C	106	GLN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	365	HIS
1	C	410	ASN
1	C	451	GLN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	537	ASN
1	D	106	GLN
1	D	123	HIS
1	D	127	GLN

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Mol	Chain	Res	Type
1	D	198	ASN
1	D	277	ASN
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	365	HIS
1	D	380	ASN
1	D	410	ASN
1	D	432	ASN
1	D	451	GLN
1	D	452	GLN
1	D	479	ASN
1	E	102	ASN
1	E	106	GLN
1	E	123	HIS
1	E	127	GLN
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	364	GLN
1	E	365	HIS
1	E	380	ASN
1	E	410	ASN
1	E	451	GLN
1	E	452	GLN
1	E	462	HIS
1	E	479	ASN
1	E	537	ASN
1	F	106	GLN
1	F	123	HIS
1	F	127	GLN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	365	HIS
1	F	380	ASN
1	F	410	ASN
1	F	432	ASN

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Mol	Chain	Res	Type
1	F	451	GLN
1	F	452	GLN
1	F	474	HIS
1	F	537	ASN
1	F	562	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 53 ligands modelled in this entry, 6 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	1571	-	3,3,3	0.89	0	2,2,2	0.27	0
4	EDO	A	1572	-	3,3,3	0.54	0	2,2,2	0.58	0
4	EDO	A	1573	-	3,3,3	0.85	0	2,2,2	0.04	0
4	EDO	A	1574	-	3,3,3	0.57	0	2,2,2	0.14	0
4	EDO	A	1575	-	3,3,3	0.40	0	2,2,2	0.70	0
4	EDO	A	1576	-	3,3,3	0.34	0	2,2,2	0.80	0
4	EDO	A	1577	-	3,3,3	0.59	0	2,2,2	0.18	0
4	EDO	A	1578	-	3,3,3	0.73	0	2,2,2	0.64	0
4	EDO	A	1579	-	3,3,3	0.73	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	1580	-	3,3,3	0.98	0	2,2,2	1.18	0
5	BBK	A	1581	-	15,15,15	8.44	2 (13%)	21,21,21	2.70	7 (33%)
6	HWU	A	1582	3	41,41,41	5.96	6 (14%)	58,62,62	1.85	14 (24%)
6	HWU	B	1571	3	41,41,41	6.21	12 (29%)	58,62,62	2.62	19 (32%)
4	EDO	B	1572	-	3,3,3	0.54	0	2,2,2	0.61	0
4	EDO	B	1573	-	3,3,3	0.30	0	2,2,2	0.36	0
4	EDO	B	1574	-	3,3,3	0.64	0	2,2,2	0.36	0
4	EDO	B	1575	-	3,3,3	0.49	0	2,2,2	0.39	0
4	EDO	B	1576	-	3,3,3	0.68	0	2,2,2	0.15	0
4	EDO	B	1577	-	3,3,3	0.30	0	2,2,2	1.17	0
4	EDO	B	1578	-	3,3,3	0.58	0	2,2,2	0.42	0
4	EDO	B	1579	-	3,3,3	0.74	0	2,2,2	0.05	0
5	BBK	B	1580	-	15,15,15	8.32	2 (13%)	21,21,21	2.48	5 (23%)
6	HWU	C	1569	3	41,41,41	7.45	8 (19%)	58,62,62	2.36	20 (34%)
6	HWU	D	1571	3	41,41,41	6.33	12 (29%)	58,62,62	2.41	17 (29%)
5	BBK	D	1572	-	15,15,15	8.78	3 (20%)	21,21,21	3.31	8 (38%)
4	EDO	D	1573	-	3,3,3	0.51	0	2,2,2	0.79	0
4	EDO	D	1574	-	3,3,3	0.84	0	2,2,2	0.50	0
4	EDO	D	1575	-	3,3,3	0.93	0	2,2,2	0.37	0
4	EDO	D	1576	-	3,3,3	0.63	0	2,2,2	0.60	0
4	EDO	D	1577	-	3,3,3	0.50	0	2,2,2	0.73	0
4	EDO	E	1570	-	3,3,3	0.78	0	2,2,2	0.37	0
4	EDO	E	1571	-	3,3,3	0.72	0	2,2,2	0.26	0
4	EDO	E	1572	-	3,3,3	0.45	0	2,2,2	0.43	0
4	EDO	E	1573	-	3,3,3	0.34	0	2,2,2	1.02	0
4	EDO	E	1574	-	3,3,3	0.40	0	2,2,2	0.88	0
4	EDO	E	1575	-	3,3,3	0.50	0	2,2,2	0.38	0
4	EDO	E	1576	-	3,3,3	0.58	0	2,2,2	0.57	0
4	EDO	E	1577	-	3,3,3	0.39	0	2,2,2	0.80	0
4	EDO	E	1578	-	3,3,3	0.44	0	2,2,2	0.72	0
4	EDO	E	1579	-	3,3,3	0.50	0	2,2,2	0.65	0
4	EDO	E	1580	-	3,3,3	0.67	0	2,2,2	0.27	0
4	EDO	E	1581	-	3,3,3	0.39	0	2,2,2	0.92	0
4	EDO	E	1582	-	3,3,3	0.40	0	2,2,2	0.34	0
4	EDO	E	1583	-	3,3,3	0.63	0	2,2,2	0.16	0
5	BBK	E	1584	-	15,15,15	8.50	2 (13%)	21,21,21	2.61	7 (33%)
6	HWU	E	1585	3	41,41,41	6.23	7 (17%)	58,62,62	2.15	15 (25%)
6	HWU	F	1571	3	41,41,41	5.86	7 (17%)	58,62,62	1.92	12 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1571	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1579	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1580	-	-	0/1/1/1	0/0/0/0
5	BBK	A	1581	-	-	2/6/26/26	0/1/1/1
6	HWU	A	1582	3	-	0/24/63/63	0/3/3/3
6	HWU	B	1571	3	-	0/24/63/63	0/3/3/3
4	EDO	B	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1579	-	-	0/1/1/1	0/0/0/0
5	BBK	B	1580	-	-	0/6/26/26	0/1/1/1
6	HWU	C	1569	3	-	1/24/63/63	0/3/3/3
6	HWU	D	1571	3	-	0/24/63/63	0/3/3/3
5	BBK	D	1572	-	-	0/6/26/26	0/1/1/1
4	EDO	D	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1570	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1571	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1574	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1575	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1576	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1577	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1578	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1579	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1580	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	1581	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1582	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1583	-	-	0/1/1/1	0/0/0/0
5	BBK	E	1584	-	-	0/6/26/26	0/1/1/1
6	HWU	E	1585	3	-	0/24/63/63	0/3/3/3
6	HWU	F	1571	3	-	0/24/63/63	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1569	HWU	C1'-S5'	-38.24	1.42	1.81
6	E	1585	HWU	C1'-S5'	-32.71	1.47	1.81
6	B	1571	HWU	C1'-S5'	-32.55	1.48	1.81
6	D	1571	HWU	C1'-S5'	-31.19	1.49	1.81
6	A	1582	HWU	C1'-S5'	-31.18	1.49	1.81
6	F	1571	HWU	C1'-S5'	-30.66	1.50	1.81
6	C	1569	HWU	C5'-S5'	-27.24	1.41	1.82
5	D	1572	BBK	C5-S5	-27.03	1.42	1.82
5	E	1584	BBK	C5-S5	-26.64	1.42	1.82
5	B	1580	BBK	C5-S5	-25.96	1.43	1.82
5	A	1581	BBK	C5-S5	-25.79	1.43	1.82
6	D	1571	HWU	C5'-S5'	-23.15	1.47	1.82
6	E	1585	HWU	C5'-S5'	-20.86	1.51	1.82
6	A	1582	HWU	C5'-S5'	-20.51	1.51	1.82
6	F	1571	HWU	C5'-S5'	-20.20	1.52	1.82
5	D	1572	BBK	C1-S5	-20.18	1.42	1.83
6	B	1571	HWU	C5'-S5'	-20.16	1.52	1.82
5	A	1581	BBK	C1-S5	-19.96	1.42	1.83
5	E	1584	BBK	C1-S5	-19.02	1.44	1.83
5	B	1580	BBK	C1-S5	-18.87	1.45	1.83
6	B	1571	HWU	O1'-C1'	5.51	1.52	1.45
6	D	1571	HWU	C4'-C5'	5.06	1.57	1.53
6	E	1585	HWU	O4B-C1B	4.50	1.46	1.41
6	E	1585	HWU	O1'-C1'	4.19	1.50	1.45
6	A	1582	HWU	O2-C2	3.97	1.27	1.21
6	D	1571	HWU	PB-O3A	-3.75	1.53	1.59
6	C	1569	HWU	C1'-C2'	3.67	1.59	1.53
6	C	1569	HWU	PA-O3A	3.55	1.66	1.59
6	C	1569	HWU	O2-C2	3.51	1.26	1.21
6	D	1571	HWU	C6'-C5'	3.49	1.55	1.52
6	D	1571	HWU	O1'-C1'	3.40	1.49	1.45
6	B	1571	HWU	C6-N1	-3.30	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1571	HWU	O2-C2	3.26	1.26	1.21
6	E	1585	HWU	PB-O3A	3.21	1.65	1.59
6	A	1582	HWU	O1'-C1'	3.10	1.49	1.45
6	D	1571	HWU	O2-C2	3.06	1.25	1.21
6	B	1571	HWU	C4'-C5'	3.02	1.55	1.53
6	F	1571	HWU	O4B-C1B	3.02	1.45	1.41
6	B	1571	HWU	C5-C4	3.00	1.41	1.37
6	D	1571	HWU	C1'-C2'	2.96	1.58	1.53
6	F	1571	HWU	C4'-C5'	2.87	1.55	1.53
6	B	1571	HWU	PB-O3A	2.85	1.64	1.59
6	F	1571	HWU	C5-C4	2.84	1.40	1.37
6	B	1571	HWU	O4B-C1B	2.81	1.44	1.41
6	E	1585	HWU	C4'-C5'	2.78	1.55	1.53
5	D	1572	BBK	C1-C2	-2.67	1.48	1.53
6	D	1571	HWU	O4B-C1B	2.65	1.44	1.41
6	D	1571	HWU	C2-N1	-2.59	1.35	1.38
6	B	1571	HWU	O5B-C5B	-2.54	1.34	1.44
6	A	1582	HWU	C6'-C5'	2.51	1.54	1.52
6	B	1571	HWU	C4-N3	-2.51	1.33	1.36
6	B	1571	HWU	PB-O2B	-2.50	1.44	1.55
6	D	1571	HWU	O5B-C5B	-2.47	1.34	1.44
6	D	1571	HWU	PA-O3A	-2.35	1.55	1.59
6	A	1582	HWU	PB-O1B	-2.20	1.43	1.51
6	C	1569	HWU	C5-C4	2.18	1.40	1.37
6	C	1569	HWU	O4B-C1B	2.14	1.43	1.41
6	B	1571	HWU	PB-O1'	2.11	1.66	1.60
6	C	1569	HWU	PB-O2B	-2.11	1.45	1.55
6	E	1585	HWU	PB-O2B	-2.09	1.45	1.55
6	F	1571	HWU	O5B-C5B	-2.06	1.36	1.44

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1571	HWU	N3-C2-N1	10.62	124.83	115.97
6	D	1571	HWU	C2-N1-C1B	9.24	124.00	118.21
5	D	1572	BBK	C1-C2-N2	-9.24	93.88	111.53
6	E	1585	HWU	N3-C2-N1	9.23	123.68	115.97
5	A	1581	BBK	C1-S5-C5	8.81	116.75	96.41
5	B	1580	BBK	C1-S5-C5	8.45	115.91	96.41
5	E	1584	BBK	C1-S5-C5	8.26	115.48	96.41
5	D	1572	BBK	O1-C1-C2	-7.13	93.37	109.27
6	F	1571	HWU	N3-C2-N1	6.90	121.73	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1569	HWU	C2-N1-C1B	6.72	122.42	118.21
6	D	1571	HWU	N3-C2-N1	6.72	121.58	115.97
5	D	1572	BBK	C1-S5-C5	6.29	110.94	96.41
6	B	1571	HWU	C1'-S5'-C5'	5.64	109.43	96.41
6	B	1571	HWU	O1'-C1'-C2'	5.55	116.37	107.12
6	B	1571	HWU	O5B-PA-O1A	5.44	130.67	109.37
6	F	1571	HWU	C1'-S5'-C5'	5.42	108.91	96.41
6	E	1585	HWU	C2-N1-C1B	5.38	121.58	118.21
6	A	1582	HWU	C1'-S5'-C5'	5.25	108.53	96.41
6	D	1571	HWU	O3A-PA-O5B	-5.23	89.06	102.91
6	C	1569	HWU	PB-O3A-PA	-5.17	117.62	131.93
6	A	1582	HWU	N3-C2-N1	5.06	120.20	115.97
6	B	1571	HWU	PB-O1'-C1'	5.04	140.90	119.58
6	D	1571	HWU	C1'-S5'-C5'	4.96	107.87	96.41
6	A	1582	HWU	PB-O1'-C1'	4.86	140.12	119.58
6	C	1569	HWU	O1'-C1'-C2'	4.63	114.84	107.12
5	A	1581	BBK	C1-C2-N2	4.60	120.31	111.53
6	D	1571	HWU	O1'-PB-O1B	-4.28	92.43	109.65
6	C	1569	HWU	C1'-S5'-C5'	4.26	106.25	96.41
6	A	1582	HWU	C6'-C5'-S5'	4.22	118.94	109.02
5	A	1581	BBK	C2-N2-C7	4.16	134.00	123.07
6	C	1569	HWU	O6'-C6'-C5'	-4.11	101.31	110.65
6	D	1571	HWU	O3'-C3'-C2'	4.06	118.08	109.59
6	C	1569	HWU	N3-C2-N1	4.02	119.32	115.97
6	E	1585	HWU	PB-O1'-C1'	3.88	135.97	119.58
6	B	1571	HWU	C4'-C5'-S5'	3.86	118.10	110.12
6	E	1585	HWU	C1'-S5'-C5'	3.81	105.21	96.41
6	A	1582	HWU	C4'-C5'-S5'	3.81	117.99	110.12
5	E	1584	BBK	C1-C2-C3	-3.81	103.98	110.07
6	C	1569	HWU	C3'-C4'-C5'	-3.76	104.36	110.95
6	F	1571	HWU	C2-N1-C1B	3.74	120.56	118.21
6	B	1571	HWU	O1'-PB-O1B	3.72	124.64	109.65
5	B	1580	BBK	C1-C2-C3	-3.71	104.13	110.07
5	D	1572	BBK	C3-C4-C5	-3.63	104.60	110.95
6	C	1569	HWU	C4B-O4B-C1B	-3.63	105.73	109.72
5	D	1572	BBK	C6-C5-S5	3.55	117.37	109.02
6	C	1569	HWU	O3A-PB-O1'	3.52	113.82	103.58
5	E	1584	BBK	C3-C2-N2	-3.52	103.13	110.60
6	D	1571	HWU	O4B-C4B-C5B	-3.51	96.92	109.37
6	C	1569	HWU	PB-O1'-C1'	3.49	134.32	119.58
6	B	1571	HWU	O3A-PA-O5B	-3.47	93.71	102.91
6	B	1571	HWU	O2A-PA-O5B	-3.34	91.68	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1569	HWU	C1'-C2'-N2'	-3.33	104.42	111.13
6	C	1569	HWU	C1'-C2'-C3'	3.33	118.65	109.61
6	E	1585	HWU	O1'-C1'-C2'	3.30	112.62	107.12
6	C	1569	HWU	O4B-C1B-N1	3.26	115.24	108.08
6	F	1571	HWU	PB-O1'-C1'	3.24	133.27	119.58
6	E	1585	HWU	C3'-C4'-C5'	-3.23	105.30	110.95
6	A	1582	HWU	O3A-PB-O1'	-3.21	94.27	103.58
6	B	1571	HWU	C4'-C3'-C2'	-3.21	105.94	110.51
6	F	1571	HWU	C4'-C5'-S5'	3.17	116.66	110.12
6	B	1571	HWU	O3A-PB-O1'	-3.16	94.40	103.58
6	C	1569	HWU	O3B-C3B-C4B	3.16	120.38	111.07
6	C	1569	HWU	O2A-PA-O3A	3.14	120.04	105.14
5	B	1580	BBK	O4-C4-C5	3.11	115.81	108.72
6	F	1571	HWU	O3A-PA-O5B	-3.10	94.69	102.91
5	E	1584	BBK	O4-C4-C5	3.08	115.75	108.72
6	F	1571	HWU	C6'-C5'-S5'	3.04	116.18	109.02
6	C	1569	HWU	C4'-C3'-C2'	-3.04	106.18	110.51
6	F	1571	HWU	O4B-C4B-C5B	-3.03	98.62	109.37
6	E	1585	HWU	O3A-PB-O1'	-3.01	94.83	103.58
5	B	1580	BBK	C2-N2-C7	2.98	130.90	123.07
6	A	1582	HWU	C2-N1-C1B	2.94	120.05	118.21
6	D	1571	HWU	PB-O3A-PA	2.86	139.86	131.93
5	E	1584	BBK	C2-N2-C7	2.83	130.51	123.07
6	D	1571	HWU	PB-O1'-C1'	2.80	131.44	119.58
6	F	1571	HWU	O2B-PB-O3A	2.79	118.38	105.14
6	F	1571	HWU	O5B-PA-O1A	2.74	120.12	109.37
6	B	1571	HWU	O3A-PB-O1B	-2.71	91.86	110.43
6	E	1585	HWU	C4'-C5'-S5'	2.68	115.66	110.12
6	D	1571	HWU	O4'-C4'-C3'	-2.67	104.39	110.36
6	D	1571	HWU	C5B-C4B-C3B	-2.67	104.51	115.19
5	A	1581	BBK	C1-C2-C3	-2.66	105.81	110.07
5	D	1572	BBK	C4-C3-C2	2.66	114.30	110.51
6	A	1582	HWU	O2B-PB-O1B	2.63	126.70	112.14
5	A	1581	BBK	C4-C5-S5	2.62	115.54	110.12
6	B	1571	HWU	O7'-C7'-N2'	2.60	127.19	121.90
6	B	1571	HWU	O4B-C4B-C5B	-2.60	100.14	109.37
6	B	1571	HWU	O4'-C4'-C3'	-2.58	104.59	110.36
6	E	1585	HWU	O3'-C3'-C2'	2.57	114.96	109.59
6	E	1585	HWU	O7'-C7'-N2'	2.57	127.13	121.90
6	A	1582	HWU	C2'-N2'-C7'	-2.56	116.36	123.07
5	B	1580	BBK	C6-C5-S5	2.55	115.02	109.02
6	E	1585	HWU	C6'-C5'-S5'	2.54	114.99	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1582	HWU	O1'-PB-O1B	-2.49	99.64	109.65
6	A	1582	HWU	C4'-C3'-C2'	-2.47	107.00	110.51
6	C	1569	HWU	C2'-C1'-S5'	2.46	119.32	111.55
6	B	1571	HWU	C2'-C1'-S5'	-2.45	103.83	111.55
6	C	1569	HWU	O4B-C4B-C3B	2.43	110.11	105.16
6	F	1571	HWU	C4'-C3'-C2'	-2.42	107.05	110.51
5	A	1581	BBK	O3-C3-C4	2.42	115.77	110.36
6	D	1571	HWU	C6'-C5'-S5'	2.42	114.71	109.02
5	E	1584	BBK	O6-C6-C5	-2.39	105.22	110.65
6	D	1571	HWU	O5B-C5B-C4B	2.37	117.68	108.96
5	D	1572	BBK	O4-C4-C5	2.36	114.12	108.72
6	C	1569	HWU	C2B-C1B-N1	-2.35	106.93	113.34
6	E	1585	HWU	O7'-C7'-C8'	-2.34	117.55	122.04
6	B	1571	HWU	C6'-C5'-S5'	2.34	114.52	109.02
5	E	1584	BBK	C4-C5-S5	2.33	114.94	110.12
6	B	1571	HWU	PB-O3A-PA	-2.32	125.51	131.93
6	E	1585	HWU	C2'-C1'-S5'	-2.31	104.27	111.55
6	A	1582	HWU	C6'-C5'-C4'	-2.26	99.69	115.05
6	F	1571	HWU	O4B-C1B-N1	2.25	113.02	108.08
6	C	1569	HWU	O5B-PA-O1A	2.22	118.06	109.37
6	A	1582	HWU	O5B-PA-O1A	-2.21	100.71	109.37
6	D	1571	HWU	O4'-C4'-C5'	2.17	113.67	108.72
6	B	1571	HWU	C4-N3-C2	-2.13	116.84	123.44
6	E	1585	HWU	C4'-C3'-C2'	-2.13	107.47	110.51
5	D	1572	BBK	O3-C3-C4	2.12	115.10	110.36
6	D	1571	HWU	C6-N1-C2	-2.12	116.56	119.51
6	D	1571	HWU	O3'-C3'-C4'	-2.11	105.64	110.36
6	E	1585	HWU	O3A-PB-O1B	-2.06	96.33	110.43
5	A	1581	BBK	C3-C2-N2	-2.05	106.25	110.60
6	D	1571	HWU	O1'-C1'-C2'	-2.02	103.75	107.12
6	A	1582	HWU	O7'-C7'-C8'	-2.01	118.19	122.04

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1581	BBK	O7-C7-N2-C2
5	A	1581	BBK	C8-C7-N2-C2
6	C	1569	HWU	PB-O1'-C1'-C2'

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	495/571 (86%)	-0.11	15 (3%)	48	48	26, 42, 70, 130	5 (1%)
1	B	495/571 (86%)	-0.17	14 (2%)	50	51	26, 40, 66, 106	5 (1%)
1	C	476/571 (83%)	1.82	173 (36%)	1	0	42, 92, 135, 168	5 (1%)
1	D	495/571 (86%)	-0.11	15 (3%)	48	48	26, 41, 66, 142	5 (1%)
1	E	495/571 (86%)	-0.27	4 (0%)	83	85	23, 36, 58, 90	5 (1%)
1	F	491/571 (85%)	0.54	78 (15%)	3	2	34, 57, 112, 140	5 (1%)
2	X	6/6 (100%)	1.17	2 (33%)	1	1	40, 73, 84, 87	0
2	Y	6/6 (100%)	2.58	4 (66%)	0	0	42, 71, 77, 83	0
All	All	2959/3438 (86%)	0.28	305 (10%)	7	6	23, 45, 109, 168	30 (1%)

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	331	TRP	10.8
1	F	547	SER	9.7
1	C	330	VAL	9.5
1	F	556	GLY	9.0
1	C	476	ALA	8.1
1	F	557	PRO	7.8
1	C	400	VAL	7.8
1	C	475	ASN	7.1
1	C	442	HIS	7.1
1	C	417	LEU	7.0
1	C	423	CYS	6.8
1	C	516	ASP	6.8
1	F	531	LEU	6.8
1	C	405	ASN	6.7
1	F	503	ALA	6.7
1	C	547	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	F	537	ASN	6.5
1	C	497	LEU	6.4
1	F	95	GLY	6.3
1	C	284	TYR	6.2
1	C	514	ARG	6.2
1	C	443	GLN	6.0
1	C	471	TYR	6.0
1	A	291	ARG	6.0
1	C	403	ALA	6.0
1	C	531	LEU	5.9
1	F	540	LEU	5.9
1	C	513	CYS	5.9
1	C	546	LYS	5.9
1	D	287	PRO	5.8
1	C	364	GLN	5.8
1	F	516	ASP	5.8
1	C	101	ARG	5.6
1	F	559	LEU	5.5
1	F	96	GLN	5.4
1	F	555	CYS	5.4
1	C	99	TYR	5.4
1	C	410	ASN	5.3
1	A	516	ASP	5.3
1	C	502	ARG	5.3
1	C	534	VAL	5.2
1	C	493	MET	5.0
1	C	177	TYR	5.0
1	F	548	GLY	5.0
1	C	89	GLY	5.0
1	C	98	PRO	5.0
1	C	440	PRO	4.9
1	C	438	ARG	4.9
1	F	94	SER	4.8
1	C	128	ARG	4.8
1	F	552	VAL	4.8
1	C	427	LYS	4.8
1	C	406	VAL	4.7
1	F	504	PRO	4.7
1	C	399	ALA	4.6
1	C	279	VAL	4.6
1	C	527	GLY	4.6
1	F	128	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	453	GLY	4.6
1	C	280	PHE	4.6
1	C	548	GLY	4.6
1	C	540	LEU	4.5
1	C	457	LEU	4.5
1	C	117	ALA	4.5
1	C	437	LEU	4.5
1	C	408	TYR	4.5
1	D	284	TYR	4.4
1	C	199	ASP	4.4
1	A	287	PRO	4.4
1	E	516	ASP	4.4
1	D	291	ARG	4.3
1	C	107	VAL	4.3
1	C	363	LYS	4.3
1	F	127	GLN	4.3
1	C	456	CYS	4.3
1	C	441	ASP	4.2
1	C	130	GLN	4.2
1	C	204	LEU	4.2
1	F	501	ASP	4.2
1	C	419	LYS	4.2
1	F	522	TRP	4.2
1	C	463	PHE	4.1
1	F	89	GLY	4.1
2	Y	6	THR	4.1
1	F	475	ASN	4.0
1	C	473	CYS	4.0
1	F	443	GLN	3.9
1	F	515	GLU	3.9
1	F	497	LEU	3.9
1	F	543	ARG	3.9
2	Y	7	CYS	3.9
1	C	454	THR	3.9
1	C	566	THR	3.9
1	B	93	ARG	3.8
1	C	421	LEU	3.8
1	F	525	ILE	3.8
1	C	522	TRP	3.8
1	C	396	TYR	3.8
1	D	516	ASP	3.8
1	C	143	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	77	ARG	3.7
1	F	93	ARG	3.7
1	C	445	ILE	3.6
1	C	329	ASP	3.6
1	F	453	GLY	3.6
1	C	113	ARG	3.6
1	F	405	ASN	3.6
1	C	401	PRO	3.6
1	C	407	PRO	3.6
1	C	439	VAL	3.6
1	F	514	ARG	3.6
1	C	385	ALA	3.5
1	C	518	SER	3.5
1	F	546	LYS	3.5
1	C	413	SER	3.5
1	C	411	ILE	3.5
1	C	412	GLN	3.5
1	C	144	PHE	3.5
1	A	295	GLY	3.5
1	E	93	ARG	3.5
1	C	100	ALA	3.4
1	F	527	GLY	3.4
1	C	422	SER	3.4
1	C	528	ASN	3.4
1	C	384	ALA	3.4
1	F	558	ALA	3.4
2	Y	5	SER	3.4
1	C	365	HIS	3.4
1	C	327	MET	3.4
1	F	535	GLY	3.4
1	C	152	LEU	3.4
1	B	371	GLY	3.4
1	C	145	HIS	3.4
1	C	111	LYS	3.4
1	D	557	PRO	3.4
1	C	182	GLU	3.4
1	C	503	ALA	3.3
1	B	516	ASP	3.3
1	C	340	PHE	3.3
1	F	442	HIS	3.3
1	C	151	ALA	3.3
1	C	97	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	284	TYR	3.3
1	C	544	THR	3.3
1	C	146	ASN	3.3
1	C	447	PHE	3.3
1	C	366	PRO	3.2
1	C	495	LEU	3.2
2	X	6	THR	3.2
1	F	465	ASP	3.2
1	C	537	ASN	3.2
1	C	316	PHE	3.1
1	B	94	SER	3.1
1	A	288	GLU	3.1
1	A	95	GLY	3.1
1	D	295	GLY	3.1
1	A	128	ARG	3.1
1	C	532	ARG	3.1
1	C	557	PRO	3.1
1	C	533	HIS	3.0
1	B	127	GLN	3.0
1	C	79	PRO	3.0
1	F	438	ARG	3.0
1	C	549	GLY	3.0
1	D	130	GLN	3.0
1	F	554	VAL	3.0
1	F	287	PRO	2.9
1	B	199	ASP	2.9
1	C	416	GLU	2.9
1	C	472	GLU	2.9
1	C	383	ARG	2.9
1	F	507	LEU	2.9
1	F	441	ASP	2.9
1	C	292	SER	2.9
1	C	555	CYS	2.9
1	C	508	ILE	2.9
1	C	91	MET	2.9
1	F	476	ALA	2.9
1	F	288	GLU	2.9
1	C	295	GLY	2.9
1	C	380	ASN	2.9
1	C	124	ASP	2.8
1	F	493	MET	2.8
1	C	435	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	150	SER	2.8
1	C	186	LEU	2.8
1	C	543	ARG	2.8
1	C	288	GLU	2.8
1	C	200	ARG	2.8
1	A	93	ARG	2.7
1	C	430	LEU	2.7
1	C	550	LEU	2.7
1	A	284	TYR	2.7
1	B	131	TRP	2.7
1	C	567	LEU	2.7
1	F	508	ILE	2.7
1	C	477	GLY	2.7
1	F	506	SER	2.7
1	C	559	LEU	2.7
1	F	454	THR	2.7
1	C	451	GLN	2.6
1	C	286	THR	2.6
1	C	404	ARG	2.6
1	F	199	ASP	2.6
1	B	130	GLN	2.6
1	D	290	ARG	2.6
1	F	544	THR	2.6
1	B	457	LEU	2.6
1	C	506	SER	2.6
1	C	397	TYR	2.6
1	C	426	PHE	2.6
1	C	485	THR	2.6
1	D	540	LEU	2.6
1	C	504	PRO	2.5
1	F	487	GLU	2.5
1	C	490	VAL	2.5
1	C	181	PRO	2.5
1	B	295	GLY	2.5
1	C	277	ASN	2.5
1	C	554	VAL	2.5
1	D	296	ASN	2.5
1	C	462	HIS	2.5
1	F	286	THR	2.5
1	C	328	MET	2.5
1	C	262	GLN	2.5
1	C	391	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	474	HIS	2.5
1	C	568	ASN	2.5
1	F	538	LEU	2.4
1	B	95	GLY	2.4
1	C	390	ASP	2.4
1	C	526	GLU	2.4
1	A	540	LEU	2.4
1	F	295	GLY	2.4
1	C	388	TRP	2.4
1	C	278	LEU	2.4
1	D	450	LEU	2.4
2	Y	8	PRO	2.4
1	F	550	LEU	2.3
1	C	517	ASP	2.3
1	C	431	GLU	2.3
1	F	391	GLU	2.3
1	A	442	HIS	2.3
1	C	536	SER	2.3
1	F	291	ARG	2.3
1	C	275	ASP	2.3
1	A	290	ARG	2.3
1	C	469	GLY	2.3
1	C	535	GLY	2.3
1	C	402	SER	2.3
1	C	428	TRP	2.3
1	A	316	PHE	2.3
1	F	523	GLU	2.3
1	F	97	ASP	2.3
1	F	457	LEU	2.3
1	C	468	VAL	2.2
1	C	108	GLU	2.2
1	C	291	ARG	2.2
1	D	457	LEU	2.2
1	C	525	ILE	2.2
1	F	363	LYS	2.2
1	D	527	GLY	2.2
1	F	526	GLU	2.2
1	B	96	GLN	2.2
1	B	128	ARG	2.2
1	F	502	ARG	2.2
1	C	386	GLU	2.2
1	C	149	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	344	GLN	2.2
1	F	419	LYS	2.2
1	F	459	THR	2.2
1	F	545	ALA	2.2
1	E	94	SER	2.2
1	F	292	SER	2.2
1	E	316	PHE	2.1
1	C	460	LEU	2.1
1	C	178	SER	2.1
1	F	450	LEU	2.1
1	F	490	VAL	2.1
1	C	505	GLY	2.1
1	A	419	LYS	2.1
1	D	531	LEU	2.1
1	A	124	ASP	2.1
1	C	481	GLU	2.1
1	F	486	LYS	2.1
1	C	564	LYS	2.1
1	F	534	VAL	2.1
1	C	512	GLY	2.1
1	C	556	GLY	2.1
1	F	541	ASP	2.1
1	C	245	ARG	2.0
1	C	362	ARG	2.0
1	D	199	ASP	2.0
2	X	5	SER	2.0
1	C	324	TYR	2.0
1	F	463	PHE	2.0
1	F	505	GLY	2.0
1	C	337	GLU	2.0
1	F	472	GLU	2.0
1	B	442	HIS	2.0
1	C	565	PHE	2.0
1	C	80	ASP	2.0
1	C	494	ASP	2.0
1	F	569	LEU	2.0
1	C	563	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	E	1578	4/4	0.22	12.47	64,64,66,82	0
4	EDO	A	1577	4/4	0.47	11.36	62,68,71,76	0
5	BBK	E	1584	15/15	0.31	8.19	96,105,117,124	0
5	BBK	D	1572	15/15	0.30	7.51	96,105,117,124	0
4	EDO	E	1580	4/4	0.39	7.44	59,70,71,76	0
4	EDO	A	1576	4/4	0.28	6.95	57,62,66,75	0
5	BBK	B	1580	15/15	0.28	6.84	69,86,120,142	0
4	EDO	E	1570	4/4	0.37	6.60	44,48,59,61	0
4	EDO	B	1576	4/4	0.20	5.71	65,69,73,76	0
4	EDO	D	1577	4/4	0.18	5.43	67,68,69,69	0
4	EDO	A	1580	4/4	0.20	4.45	45,52,57,59	0
4	EDO	A	1573	4/4	0.20	4.43	56,68,70,70	0
4	EDO	E	1576	4/4	0.17	4.24	68,68,69,69	0
4	EDO	E	1577	4/4	0.25	4.00	61,61,64,68	0
4	EDO	B	1573	4/4	0.23	3.87	40,41,42,48	0
4	EDO	A	1579	4/4	0.19	3.84	51,52,54,64	0
4	EDO	E	1573	4/4	0.24	2.93	49,58,60,71	0
4	EDO	B	1575	4/4	0.28	2.92	66,68,69,69	0
4	EDO	A	1572	4/4	0.23	2.72	57,66,67,69	0
4	EDO	A	1571	4/4	0.23	2.48	43,46,46,52	0
4	EDO	D	1576	4/4	0.17	2.36	39,43,45,49	0
4	EDO	E	1581	4/4	0.17	2.22	53,56,60,68	0
4	EDO	B	1578	4/4	0.28	2.08	55,58,62,69	0
4	EDO	A	1578	4/4	0.20	1.95	38,45,48,63	0
4	EDO	E	1583	4/4	0.14	1.91	58,61,62,68	0
4	EDO	D	1573	4/4	0.13	1.71	38,40,40,45	0
4	EDO	A	1574	4/4	0.14	1.61	51,52,54,57	0
4	EDO	B	1577	4/4	0.19	1.48	42,43,48,57	0
4	EDO	E	1572	4/4	0.21	1.39	38,45,48,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	BBK	A	1581	15/15	0.23	1.36	69,86,120,142	0
4	EDO	D	1574	4/4	0.15	1.15	49,50,52,58	0
4	EDO	B	1579	4/4	0.12	0.47	41,48,56,56	0
4	EDO	D	1575	4/4	0.18	0.37	60,63,68,70	0
4	EDO	E	1574	4/4	0.19	0.12	62,68,68,75	0
6	HWU	F	1571	39/39	0.11	0.09	38,44,55,60	0
4	EDO	E	1575	4/4	0.15	-0.02	64,69,69,76	0
6	HWU	D	1571	39/39	0.11	-0.03	24,35,45,46	0
6	HWU	B	1571	39/39	0.12	-0.06	30,36,44,49	0
4	EDO	A	1575	4/4	0.10	-0.09	53,55,57,59	0
6	HWU	A	1582	39/39	0.11	-0.13	26,34,45,48	0
4	EDO	E	1582	4/4	0.11	-0.18	47,48,51,56	0
4	EDO	B	1574	4/4	0.10	-0.29	40,40,42,45	0
6	HWU	E	1585	39/39	0.11	-0.34	26,36,54,58	0
4	EDO	E	1571	4/4	0.12	-0.44	38,46,47,50	0
4	EDO	E	1579	4/4	0.10	-0.57	43,44,52,53	0
6	HWU	C	1569	39/39	0.17	-0.61	51,76,89,92	0
4	EDO	B	1572	4/4	0.08	-1.14	34,35,35,42	0
3	MN	A	1570	1/1	0.07	-1.34	27,27,27,27	0
3	MN	B	1570	1/1	0.08	-1.56	33,33,33,33	0
3	MN	D	1570	1/1	0.07	-1.84	29,29,29,29	0
3	MN	E	1586	1/1	0.07	-2.37	26,26,26,26	0
3	MN	C	1570	1/1	0.03	-2.52	59,59,59,59	0
3	MN	F	1570	1/1	0.03	-9.30	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.