



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 08:15 PM EDT

PDB ID : 1EQ2  
Title : THE CRYSTAL STRUCTURE OF ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE  
Authors : Deacon, A.M.; Ni, Y.S.; Coleman Jr., W.G.; Ealick, S.E.  
Deposited on : unknown  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

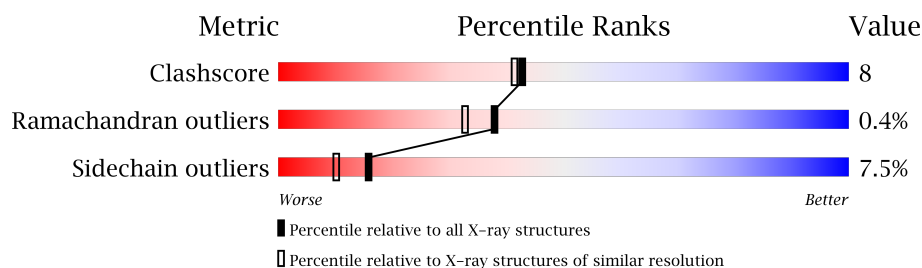
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.








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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	 69% 16% • 12%
1	B	310	 79% 15% • • •
1	C	310	 69% 17% • 12%
1	D	310	 77% 19% • •
1	E	310	 76% 17% • •
1	F	310	 75% 22% • •
1	G	310	 83% 14% • •

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Mol	Chain	Length	Quality of chain
1	H	310	
1	I	310	
1	J	310	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	G	2406	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25435 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 ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2150	1375	349	417	9			
1	B	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	C	272	Total	C	N	O	S	0	0	0
			2160	1385	348	418	9			
1	D	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	E	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	F	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	G	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	H	297	Total	C	N	O	S	0	0	0
			2360	1511	381	459	9			
1	I	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	J	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			

There are 10 discrepancies between the modelled and reference sequences:

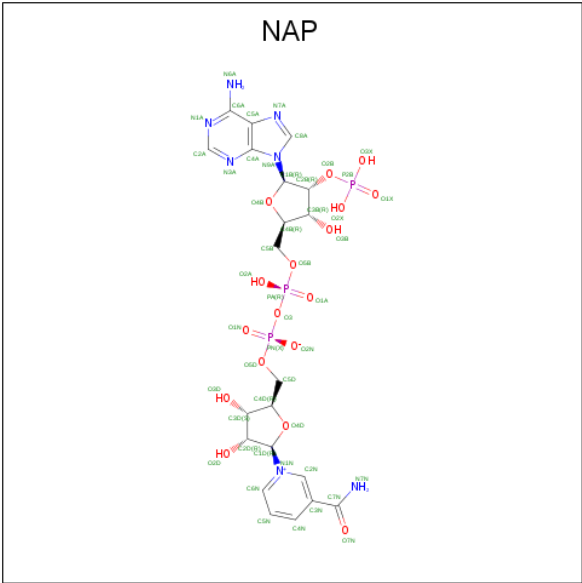
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
B	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
C	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
D	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
E	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
F	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
G	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
H	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910
I	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910

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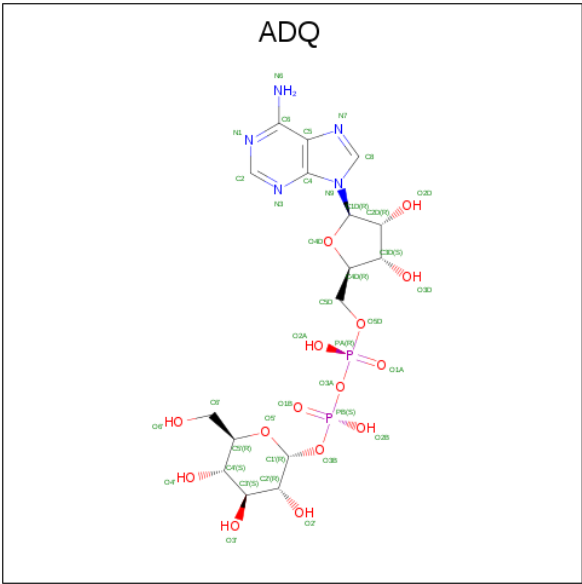
Chain	Residue	Modelled	Actual	Comment	Reference
J	78	CSO	CYS	MODIFIED RESIDUE	UNP P67910

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: ADQ) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



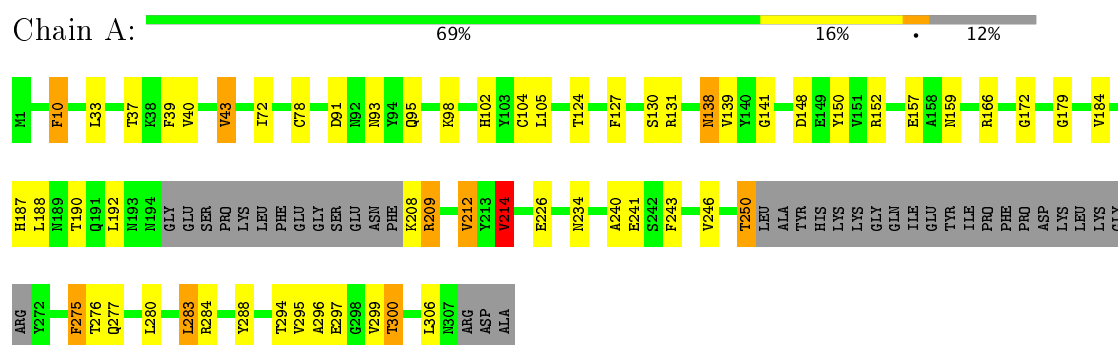
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	119	Total 119	O 119	0	0
4	C	82	Total 82	O 82	0	0
4	D	118	Total 118	O 118	0	0
4	E	105	Total 105	O 105	0	0
4	F	106	Total 106	O 106	0	0
4	G	118	Total 118	O 118	0	0
4	H	114	Total 114	O 114	0	0
4	I	123	Total 123	O 123	0	0
4	J	101	Total 101	O 101	0	0

### 3 Residue-property plots

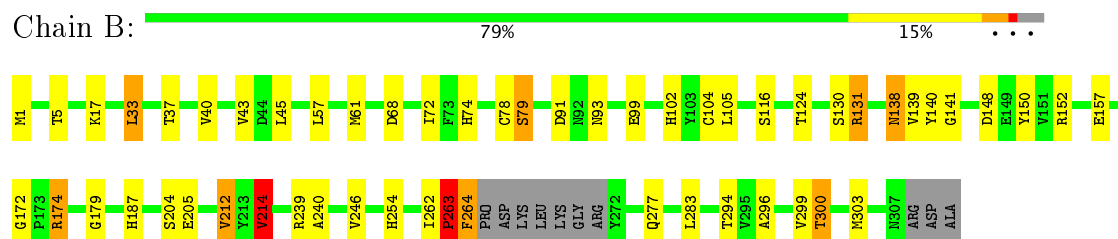
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

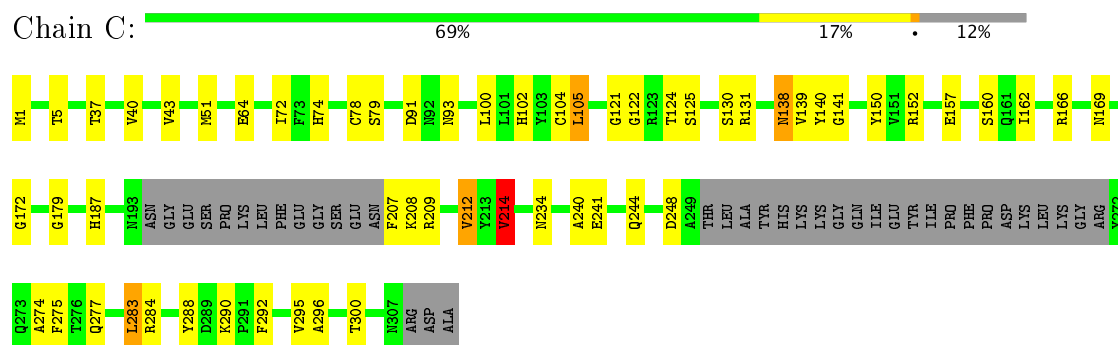
#### • Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE



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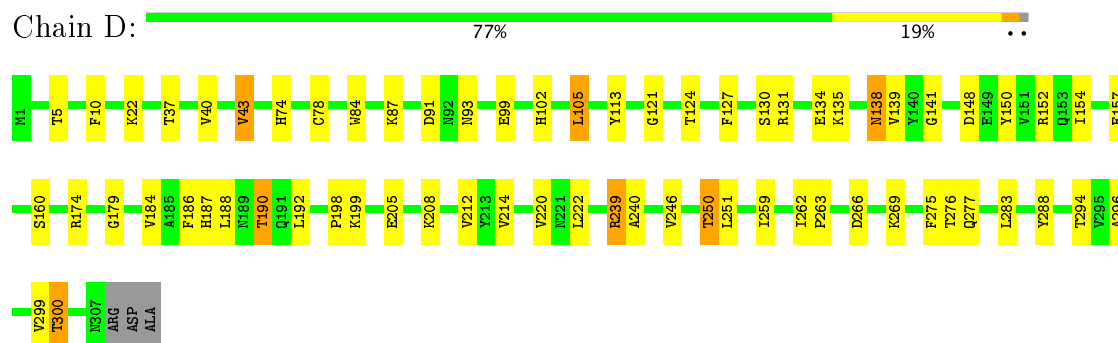


#### • Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

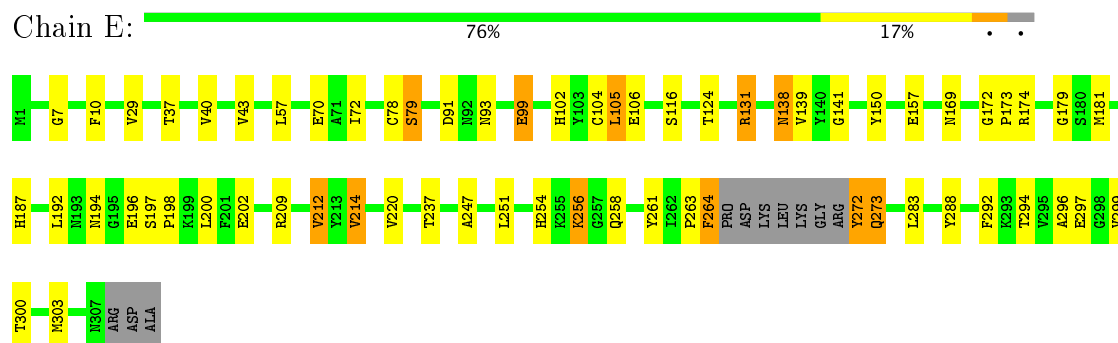


#### • Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

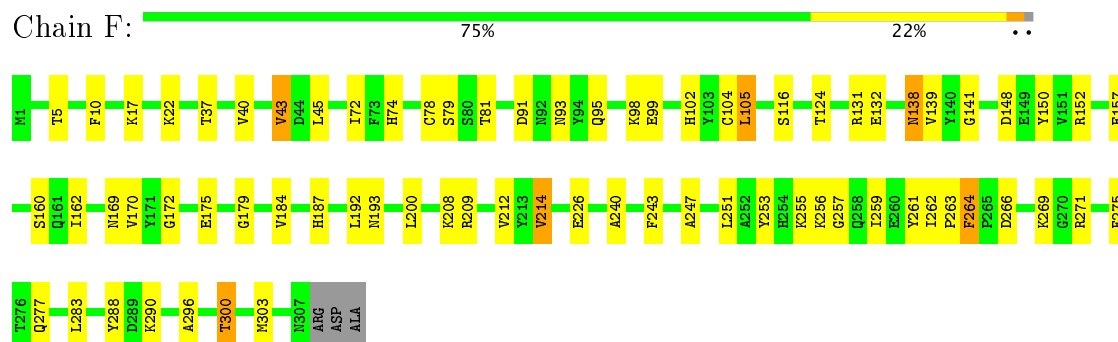




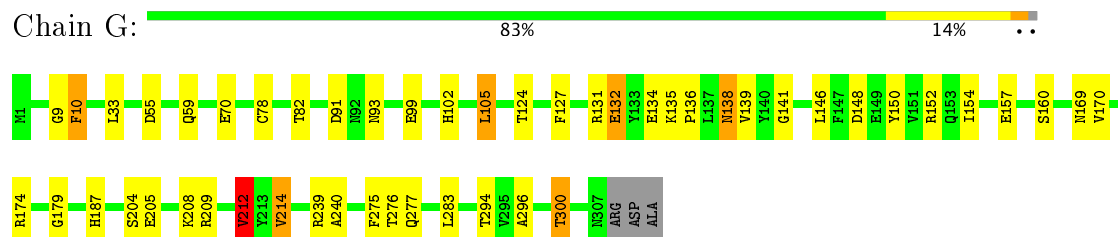
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

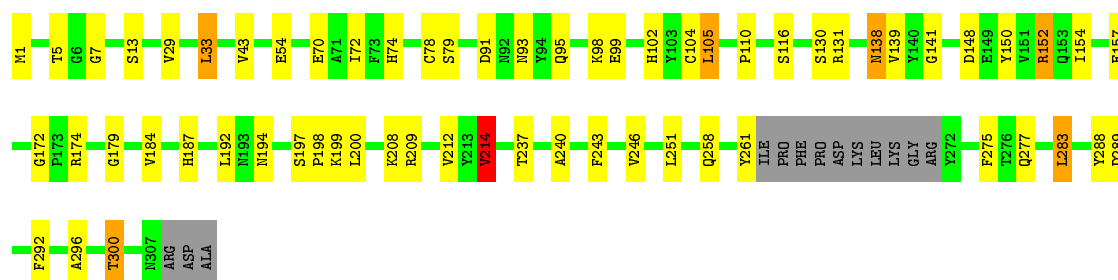


• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE



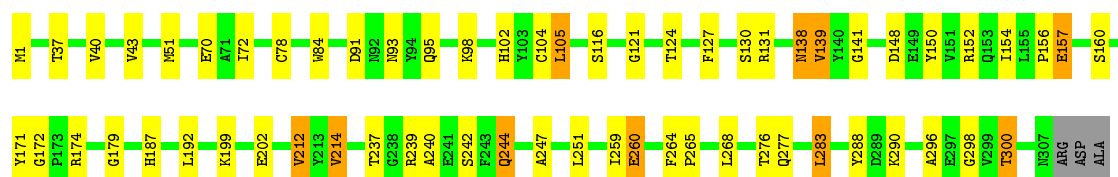
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE





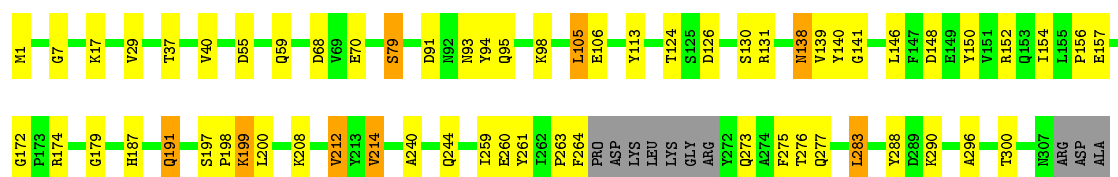
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain I: 79% 17%



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain J: 77% 17%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.46 Å   109.76 Å   181.54 Å 90.00°   91.04°   90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (20.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.212 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, NAP, ADQ

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	0.59	0/2188	0.70	2/2958 (0.1%)
1	B	0.59	0/2434	0.73	4/3290 (0.1%)
1	C	0.63	0/2200	0.74	2/2973 (0.1%)
1	D	0.58	0/2492	0.74	0/3368
1	E	0.60	0/2434	0.74	2/3290 (0.1%)
1	F	0.59	0/2492	0.72	0/3368
1	G	0.59	0/2492	0.73	1/3368 (0.0%)
1	H	0.61	0/2406	0.73	2/3251 (0.1%)
1	I	0.60	0/2492	0.73	1/3368 (0.0%)
1	J	0.59	0/2434	0.73	2/3290 (0.1%)
All	All	0.60	0/24064	0.73	16/32524 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	N-CA-C	-5.76	95.45	111.00
1	J	212	VAL	CB-CA-C	-5.64	100.68	111.40
1	C	214	VAL	CB-CA-C	-5.64	100.68	111.40
1	A	212	VAL	CB-CA-C	-5.63	100.70	111.40
1	I	212	VAL	CB-CA-C	-5.62	100.73	111.40
1	A	214	VAL	CB-CA-C	-5.51	100.93	111.40
1	B	212	VAL	CB-CA-C	-5.44	101.06	111.40
1	H	152	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	212	VAL	CB-CA-C	-5.35	101.23	111.40
1	H	214	VAL	CB-CA-C	-5.27	101.39	111.40
1	J	174	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	E	212	VAL	CB-CA-C	-5.15	101.61	111.40
1	B	263	PRO	N-CA-C	5.14	125.47	112.10
1	E	273	GLN	N-CA-C	-5.05	97.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	VAL	CB-CA-C	-5.04	101.83	111.40
1	G	212	VAL	CB-CA-C	-5.02	101.86	111.40

There are no chirality outliers.

There are no planarity outliers.

## 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	2150	0	2045	36	0
1	B	2386	0	2272	29	0
1	C	2160	0	2056	30	0
1	D	2442	0	2337	39	0
1	E	2386	0	2272	35	0
1	F	2442	0	2337	42	0
1	G	2442	0	2337	38	0
1	H	2360	0	2245	36	0
1	I	2442	0	2337	34	0
1	J	2386	0	2271	34	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	0	0
3	A	27	0	12	3	0
3	B	38	0	23	2	0
3	C	27	0	12	2	0
3	D	38	0	23	0	0
3	E	27	0	12	3	0
3	F	38	0	23	3	0
3	G	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	27	0	12	1	0
3	I	27	0	12	3	0
3	J	27	0	12	0	0
4	A	70	0	0	4	0
4	B	119	0	0	5	0
4	C	82	0	0	5	0
4	D	118	0	0	4	0
4	E	105	0	0	2	0
4	F	106	0	0	6	0
4	G	118	0	0	3	0
4	H	114	0	0	4	0
4	I	123	0	0	6	0
4	J	101	0	0	7	0
All	All	25435	0	22912	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (368) 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)
3:A:2500:ADQ:H8	3:A:2500:ADQ:H5'1	1.30	1.13
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:H8	1.39	1.04
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:H8	1.41	1.01
3:C:2502:ADQ:H8	3:C:2502:ADQ:H5'1	1.40	1.00
1:F:296:ALA:O	1:F:300:THR:HG23	1.64	0.95
1:A:296:ALA:O	1:A:300:THR:HG23	1.69	0.93
1:D:296:ALA:O	1:D:300:THR:HG23	1.69	0.93
1:H:296:ALA:O	1:H:300:THR:HG23	1.70	0.92
1:J:296:ALA:O	1:J:300:THR:HG23	1.70	0.91
1:B:296:ALA:O	1:B:300:THR:HG23	1.71	0.90
1:G:296:ALA:O	1:G:300:THR:HG23	1.72	0.88
1:E:296:ALA:O	1:E:300:THR:HG23	1.76	0.84
1:D:239:ARG:HH22	1:D:294:THR:HA	1.41	0.84
1:D:246:VAL:O	1:D:250:THR:HG23	1.80	0.81
1:F:169:ASN:HD21	1:F:209:ARG:HH11	1.28	0.81
1:C:169:ASN:HD21	1:C:209:ARG:HH11	1.28	0.81
1:H:78:CSO:H	1:H:93:ASN:HD21	1.31	0.79
1:J:240:ALA:H	1:J:277:GLN:HE21	1.31	0.78
1:B:240:ALA:H	1:B:277:GLN:HE21	1.30	0.77
1:C:296:ALA:O	1:C:300:THR:HG23	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:ALA:O	1:I:300:THR:HG23	1.84	0.77
1:I:78:CSO:H	1:I:93:ASN:HD21	1.34	0.76
1:D:78:CSO:H	1:D:93:ASN:HD21	1.33	0.75
1:C:78:CSO:H	1:C:93:ASN:HD21	1.34	0.75
1:B:78:CSO:H	1:B:93:ASN:HD21	1.36	0.74
1:E:263:PRO:O	1:E:264:PHE:HB2	1.86	0.74
3:B:2501:ADQ:H5'1	3:B:2501:ADQ:H8	1.69	0.74
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:C8	2.16	0.74
1:H:240:ALA:H	1:H:277:GLN:HE21	1.35	0.73
1:H:300:THR:HG22	4:H:979:HOH:O	1.89	0.73
1:F:300:THR:HG22	4:F:798:HOH:O	1.90	0.72
1:G:138:ASN:HD22	1:G:141:GLY:H	1.36	0.71
1:B:138:ASN:ND2	1:B:141:GLY:H	1.88	0.71
1:E:78:CSO:H	1:E:93:ASN:HD21	1.38	0.71
3:E:2504:ADQ:H8	3:E:2504:ADQ:C5D	2.22	0.70
1:I:138:ASN:ND2	1:I:141:GLY:H	1.88	0.70
1:A:138:ASN:ND2	1:A:141:GLY:H	1.89	0.69
1:F:138:ASN:ND2	1:F:141:GLY:H	1.89	0.69
1:I:268:LEU:HD11	3:I:2508:ADQ:H5'2	1.73	0.69
1:G:138:ASN:ND2	1:G:141:GLY:H	1.88	0.69
1:G:240:ALA:H	1:G:277:GLN:HE21	1.37	0.69
1:E:138:ASN:ND2	1:E:141:GLY:H	1.90	0.69
1:H:138:ASN:ND2	1:H:141:GLY:H	1.91	0.68
1:I:290:LYS:HB3	4:I:1653:HOH:O	1.92	0.68
1:I:138:ASN:HD22	1:I:141:GLY:H	1.41	0.68
1:B:262:ILE:HG23	1:B:263:PRO:HD2	1.74	0.68
1:D:138:ASN:HD22	1:D:141:GLY:H	1.40	0.67
1:A:159:ASN:HB3	4:A:1472:HOH:O	1.95	0.67
1:A:72:ILE:HD12	1:A:104:CYS:SG	2.35	0.67
1:B:300:THR:HG22	4:B:898:HOH:O	1.94	0.67
1:F:262:ILE:HG23	1:F:263:PRO:HD2	1.77	0.67
1:D:300:THR:HG22	4:D:1467:HOH:O	1.94	0.65
1:D:190:THR:HG22	4:D:901:HOH:O	1.97	0.65
1:F:78:CSO:H	1:F:93:ASN:HD21	1.44	0.65
1:A:138:ASN:HD22	1:A:141:GLY:H	1.45	0.65
3:C:2502:ADQ:C8	3:C:2502:ADQ:H5'1	2.21	0.64
1:F:240:ALA:H	1:F:277:GLN:HE21	1.45	0.64
1:A:78:CSO:H	1:A:93:ASN:HD21	1.46	0.63
3:E:2504:ADQ:H8	3:E:2504:ADQ:H5'1	1.80	0.63
1:G:78:CSO:H	1:G:93:ASN:HD21	1.44	0.63
1:C:51:MET:HE2	4:C:1516:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:ARG:NH1	4:H:852:HOH:O	2.33	0.61
1:H:72:ILE:HD12	1:H:104:CYS:SG	2.40	0.61
1:J:37:THR:O	1:J:40:VAL:HG22	1.99	0.61
1:C:138:ASN:HD22	1:C:141:GLY:H	1.49	0.61
1:G:9:GLY:HA3	2:G:2406:NAP:H52A	1.82	0.61
1:I:260:GLU:HG3	1:I:260:GLU:O	2.00	0.60
1:D:138:ASN:ND2	1:D:141:GLY:H	1.99	0.60
1:A:240:ALA:H	1:A:277:GLN:HE21	1.49	0.59
3:B:2501:ADQ:C8	3:B:2501:ADQ:H5'1	2.32	0.59
1:H:138:ASN:HD22	1:H:141:GLY:H	1.48	0.59
1:I:240:ALA:H	1:I:277:GLN:HE21	1.49	0.59
1:E:138:ASN:HD22	1:E:141:GLY:H	1.48	0.59
1:H:13:SER:OG	1:H:174:ARG:HD3	2.02	0.59
1:J:7:GLY:HA3	1:J:29:VAL:HG13	1.84	0.59
1:C:283:LEU:HD22	1:C:288:TYR:HB3	1.84	0.58
1:F:37:THR:O	1:F:40:VAL:HG22	2.02	0.58
1:D:148:ASP:O	1:D:152:ARG:HG3	2.02	0.58
1:J:138:ASN:ND2	1:J:141:GLY:H	2.00	0.58
1:B:72:ILE:HD12	1:B:104:CYS:SG	2.43	0.58
1:F:138:ASN:HD22	1:F:141:GLY:H	1.50	0.58
1:C:72:ILE:HD12	1:C:104:CYS:SG	2.44	0.58
1:C:152:ARG:HD3	4:C:1634:HOH:O	2.04	0.58
1:C:240:ALA:H	1:C:277:GLN:HE21	1.50	0.58
1:E:272:TYR:O	1:E:273:GLN:HG3	2.04	0.58
1:H:197:SER:OG	1:H:199:LYS:HE3	2.04	0.58
1:B:138:ASN:HD22	1:B:141:GLY:H	1.51	0.57
1:B:254:HIS:HD2	4:B:1497:HOH:O	1.86	0.57
1:E:294:THR:OG1	1:E:297:GLU:HG3	2.04	0.57
1:H:192:LEU:HD11	1:H:251:LEU:CD2	2.33	0.57
1:A:190:THR:HG23	4:A:1230:HOH:O	2.03	0.57
1:D:239:ARG:NH2	1:D:294:THR:HA	2.18	0.57
1:H:289:ASP:HB3	4:H:1534:HOH:O	2.04	0.57
1:I:199:LYS:HG2	1:I:260:GLU:HG2	1.85	0.57
1:I:290:LYS:HG2	4:I:1455:HOH:O	2.05	0.57
1:C:138:ASN:ND2	1:C:141:GLY:H	2.01	0.57
3:F:2505:ADQ:C5D	3:F:2505:ADQ:H8	2.25	0.56
1:A:37:THR:O	1:A:40:VAL:HG22	2.05	0.56
1:G:148:ASP:O	1:G:152:ARG:HG3	2.06	0.56
1:F:169:ASN:ND2	1:F:209:ARG:HH11	1.99	0.56
1:E:256:LYS:NZ	1:E:256:LYS:HB2	2.21	0.56
1:D:174:ARG:HD2	4:D:747:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:O	1:E:261:TYR:HA	2.06	0.56
1:J:150:TYR:HB2	4:J:1538:HOH:O	2.06	0.56
1:C:207:PHE:HA	1:C:274:ALA:O	2.06	0.56
1:H:192:LEU:HD21	1:H:198:PRO:HG3	1.89	0.55
1:J:138:ASN:HD22	1:J:141:GLY:H	1.52	0.55
1:G:174:ARG:HD2	4:G:700:HOH:O	2.06	0.55
1:J:197:SER:O	1:J:199:LYS:HG3	2.07	0.55
1:A:10:PHE:HB3	2:A:2400:NAP:O2N	2.06	0.55
1:F:105:LEU:HD11	1:F:162:ILE:HD11	1.87	0.55
1:G:240:ALA:N	1:G:277:GLN:HE21	2.04	0.55
1:H:148:ASP:O	1:H:152:ARG:HG3	2.06	0.55
1:I:148:ASP:O	1:I:152:ARG:HG3	2.07	0.55
1:I:283:LEU:HD22	1:I:288:TYR:HB3	1.89	0.55
1:C:37:THR:O	1:C:40:VAL:HG22	2.07	0.55
1:G:169:ASN:HD21	1:G:209:ARG:HH11	1.55	0.55
1:A:166:ARG:HB2	1:A:234:ASN:HA	1.89	0.54
1:F:72:ILE:HD12	1:F:104:CYS:SG	2.48	0.54
1:F:259:ILE:HD12	4:F:1513:HOH:O	2.06	0.54
1:I:37:THR:O	1:I:40:VAL:HG22	2.07	0.54
1:I:51:MET:HG3	4:I:755:HOH:O	2.06	0.54
1:B:239:ARG:HH21	1:B:294:THR:HA	1.72	0.54
1:G:135:LYS:HD3	4:J:1594:HOH:O	2.07	0.54
1:G:208:LYS:O	1:G:275:PHE:HA	2.07	0.54
1:F:81:THR:HG23	4:F:1210:HOH:O	2.07	0.54
1:I:174:ARG:HD2	4:I:808:HOH:O	2.08	0.54
1:F:169:ASN:HD21	1:F:209:ARG:NH1	2.01	0.53
1:B:57:LEU:O	1:B:61:MET:HG3	2.08	0.53
1:G:300:THR:HG22	4:G:1022:HOH:O	2.08	0.53
1:J:273:GLN:NE2	1:J:276:THR:HG22	2.23	0.53
1:J:55:ASP:O	1:J:59:GLN:HG3	2.09	0.53
1:F:192:LEU:HD11	1:F:251:LEU:HD22	1.90	0.53
1:H:200:LEU:O	1:H:261:TYR:HA	2.08	0.53
1:I:105:LEU:HD21	1:I:154:ILE:HG21	1.91	0.53
1:B:17:LYS:HE3	4:B:1402:HOH:O	2.09	0.52
1:G:102:HIS:HE1	1:G:150:TYR:OH	1.92	0.52
1:C:179:GLY:O	1:C:187:HIS:HE1	1.93	0.52
1:I:102:HIS:HE1	1:I:150:TYR:OH	1.93	0.52
1:B:148:ASP:O	1:B:152:ARG:HG3	2.10	0.52
1:D:113:TYR:HB2	4:D:1434:HOH:O	2.10	0.52
1:F:263:PRO:O	1:F:264:PHE:HB2	2.09	0.52
1:A:102:HIS:HE1	1:A:150:TYR:OH	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.24	0.52
1:B:240:ALA:N	1:B:277:GLN:HE21	2.02	0.52
1:E:7:GLY:HA3	1:E:29:VAL:HG13	1.91	0.52
1:F:40:VAL:HA	1:F:43:VAL:HG22	1.92	0.51
1:G:179:GLY:O	1:G:187:HIS:HE1	1.94	0.51
1:F:256:LYS:HG2	1:F:257:GLY:N	2.25	0.51
3:A:2500:ADQ:C8	3:A:2500:ADQ:H5'1	2.22	0.51
1:C:208:LYS:O	1:C:275:PHE:HA	2.11	0.51
1:E:192:LEU:HD13	1:E:254:HIS:CG	2.46	0.51
1:A:172:GLY:HA3	1:A:214:VAL:HG22	1.93	0.51
1:F:187:HIS:HD2	4:F:1262:HOH:O	1.94	0.51
1:F:179:GLY:O	1:F:187:HIS:HE1	1.93	0.51
1:E:102:HIS:O	1:E:106:GLU:HG3	2.11	0.50
1:G:240:ALA:H	1:G:277:GLN:NE2	2.06	0.50
1:J:300:THR:HG22	4:J:1040:HOH:O	2.11	0.50
1:B:174:ARG:HD2	4:B:969:HOH:O	2.10	0.50
1:C:121:GLY:HA2	4:C:1017:HOH:O	2.12	0.50
1:I:172:GLY:HA3	1:I:214:VAL:HG22	1.93	0.50
1:J:208:LYS:O	1:J:275:PHE:HA	2.12	0.50
1:D:102:HIS:HE1	1:D:150:TYR:OH	1.94	0.50
1:F:5:THR:OG1	1:F:74:HIS:HA	2.12	0.50
1:D:240:ALA:H	1:D:277:GLN:HE21	1.60	0.49
1:A:246:VAL:O	1:A:250:THR:HG23	2.13	0.49
1:F:152:ARG:HD3	4:F:1237:HOH:O	2.11	0.49
1:H:283:LEU:HD22	1:H:288:TYR:HB3	1.94	0.49
1:J:240:ALA:N	1:J:277:GLN:HE21	2.06	0.49
1:C:102:HIS:HE1	1:C:150:TYR:OH	1.95	0.49
1:D:208:LYS:O	1:D:275:PHE:HA	2.12	0.49
3:A:2500:ADQ:C5D	3:A:2500:ADQ:H8	2.22	0.49
1:F:148:ASP:O	1:F:152:ARG:HG3	2.13	0.49
1:F:10:PHE:CD1	1:F:175:GLU:HB3	2.48	0.49
1:B:179:GLY:O	1:B:187:HIS:HE1	1.95	0.49
1:E:179:GLY:O	1:E:187:HIS:HE1	1.95	0.49
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:C8	2.26	0.49
1:H:172:GLY:HA3	1:H:214:VAL:HG22	1.93	0.49
1:I:157:GLU:HB3	4:I:1496:HOH:O	2.12	0.49
1:A:283:LEU:HD22	1:A:288:TYR:HB3	1.95	0.48
1:J:172:GLY:HA3	1:J:214:VAL:HG22	1.95	0.48
1:J:288:TYR:CZ	1:J:290:LYS:HB2	2.48	0.48
1:C:172:GLY:HA3	1:C:214:VAL:HG22	1.96	0.48
1:D:102:HIS:CE1	1:D:150:TYR:OH	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:TYR:CZ	1:F:290:LYS:HB2	2.48	0.48
1:I:121:GLY:HA2	4:I:1159:HOH:O	2.12	0.48
1:A:296:ALA:HB3	4:A:994:HOH:O	2.14	0.48
1:D:87:LYS:HE2	4:E:1358:HOH:O	2.13	0.48
1:J:261:TYR:CD1	1:J:261:TYR:N	2.81	0.48
1:F:200:LEU:O	1:F:261:TYR:HA	2.13	0.48
1:H:198:PRO:HD2	1:H:258:GLN:O	2.14	0.48
1:A:184:VAL:O	1:A:188:LEU:HG	2.13	0.48
1:H:209:ARG:NH1	3:H:2507:ADQ:O2B	2.45	0.48
1:J:105:LEU:HD21	1:J:154:ILE:HG21	1.95	0.48
1:G:136:PRO:HD2	4:J:1524:HOH:O	2.13	0.47
1:G:82:THR:HG22	4:G:985:HOH:O	2.12	0.47
1:A:208:LYS:O	1:A:275:PHE:HA	2.13	0.47
1:H:70:GLU:O	1:H:110:PRO:HD2	2.14	0.47
1:F:200:LEU:HD11	1:F:247:ALA:HB2	1.96	0.47
1:H:179:GLY:O	1:H:187:HIS:HE1	1.96	0.47
1:E:37:THR:O	1:E:40:VAL:HG22	2.14	0.47
1:J:283:LEU:HD22	1:J:288:TYR:HB3	1.97	0.47
1:C:125:SER:HA	4:C:1556:HOH:O	2.14	0.47
1:D:250:THR:HG22	1:D:299:VAL:HG11	1.97	0.47
1:E:102:HIS:HE1	1:E:150:TYR:OH	1.98	0.47
1:G:239:ARG:HA	1:G:277:GLN:HE21	1.79	0.47
1:I:199:LYS:HG2	1:I:260:GLU:CG	2.45	0.47
1:J:95:GLN:NE2	1:J:98:LYS:HE2	2.30	0.47
1:A:102:HIS:CE1	1:A:150:TYR:OH	2.68	0.47
1:D:37:THR:O	1:D:40:VAL:HG22	2.15	0.47
1:F:253:TYR:CD2	1:F:303:MET:HB3	2.50	0.47
1:C:292:PHE:HD1	4:C:1544:HOH:O	1.96	0.47
1:D:186:PHE:O	1:D:190:THR:HG23	2.14	0.46
1:D:192:LEU:HD11	1:D:251:LEU:HD22	1.97	0.46
1:D:179:GLY:O	1:D:187:HIS:HE1	1.97	0.46
1:J:191:GLN:HG2	1:J:197:SER:O	2.15	0.46
1:D:22:LYS:HD2	1:D:222:LEU:CD1	2.46	0.46
1:D:5:THR:OG1	1:D:74:HIS:HA	2.14	0.46
1:G:102:HIS:CE1	1:G:150:TYR:OH	2.68	0.46
1:F:263:PRO:O	1:F:264:PHE:CB	2.63	0.46
1:B:246:VAL:HG11	4:B:1658:HOH:O	2.15	0.46
1:A:300:THR:HG22	4:A:1525:HOH:O	2.15	0.46
1:D:266:ASP:HA	1:D:269:LYS:HG3	1.97	0.46
1:H:102:HIS:CE1	1:H:150:TYR:OH	2.68	0.46
1:D:105:LEU:HD21	1:D:154:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLU:OE1	1:D:152:ARG:NH2	2.49	0.46
1:D:199:LYS:HB3	1:D:262:ILE:HG12	1.96	0.46
1:E:173:PRO:O	1:E:174:ARG:HB2	2.15	0.46
1:E:202:GLU:OE1	1:E:263:PRO:HA	2.16	0.46
1:G:239:ARG:NH2	1:G:294:THR:HG22	2.31	0.46
1:C:244:GLN:NE2	1:C:248:ASP:OD1	2.48	0.46
1:J:264:PHE:HD2	4:J:1365:HOH:O	1.99	0.45
1:A:250:THR:HG22	1:A:299:VAL:HG11	1.97	0.45
1:C:288:TYR:CE1	1:C:290:LYS:HE2	2.51	0.45
1:E:116:SER:HB2	2:E:2404:NAP:H6N	1.99	0.45
1:H:105:LEU:HD21	1:H:154:ILE:HG21	1.98	0.45
1:H:192:LEU:CD2	1:H:198:PRO:HG3	2.46	0.45
1:I:127:PHE:CZ	1:I:276:THR:HA	2.51	0.45
1:F:95:GLN:NE2	1:F:98:LYS:HE2	2.31	0.45
1:H:5:THR:OG1	1:H:74:HIS:HA	2.17	0.45
1:I:95:GLN:NE2	1:I:98:LYS:HE2	2.31	0.45
1:C:5:THR:OG1	1:C:74:HIS:HA	2.17	0.45
1:E:247:ALA:O	1:E:251:LEU:HD13	2.16	0.45
1:E:102:HIS:CE1	1:E:150:TYR:OH	2.69	0.45
1:E:131:ARG:HD3	1:E:131:ARG:O	2.17	0.45
1:H:197:SER:HA	1:H:198:PRO:HD3	1.86	0.45
1:J:179:GLY:O	1:J:187:HIS:HE1	2.00	0.45
1:A:148:ASP:O	1:A:152:ARG:HG3	2.17	0.45
1:A:95:GLN:NE2	1:A:98:LYS:HE2	2.32	0.45
1:B:172:GLY:HA3	1:B:214:VAL:HG22	1.99	0.45
1:H:237:THR:HG22	1:H:292:PHE:HB3	1.98	0.45
1:H:102:HIS:HE1	1:H:150:TYR:OH	2.00	0.44
1:B:172:GLY:HA3	1:B:214:VAL:CG2	2.47	0.44
1:E:220:VAL:HG22	1:E:288:TYR:CZ	2.52	0.44
1:H:246:VAL:HG11	4:H:1553:HOH:O	2.17	0.44
1:H:7:GLY:HA3	1:H:29:VAL:HG13	1.99	0.44
1:F:255:LYS:HA	1:F:255:LYS:HD3	1.79	0.44
1:J:148:ASP:O	1:J:152:ARG:HG3	2.16	0.44
1:I:72:ILE:HD12	1:I:104:CYS:SG	2.57	0.44
1:E:169:ASN:HD21	1:E:209:ARG:HH11	1.64	0.44
1:F:172:GLY:HA3	1:F:214:VAL:HG22	1.99	0.44
1:B:131:ARG:O	1:B:131:ARG:HD3	2.18	0.44
1:D:198:PRO:HB2	1:D:259:ILE:HD13	2.00	0.44
1:J:93:ASN:N	1:J:93:ASN:HD22	2.15	0.44
1:I:192:LEU:HD11	1:I:251:LEU:HD12	2.00	0.44
1:A:188:LEU:O	1:A:192:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:VAL:HG22	1:D:288:TYR:CZ	2.53	0.43
1:E:72:ILE:HD12	1:E:104:CYS:SG	2.58	0.43
1:C:102:HIS:CE1	1:C:150:TYR:OH	2.71	0.43
1:E:172:GLY:HA3	1:E:214:VAL:HG22	2.00	0.43
1:J:172:GLY:HA3	1:J:214:VAL:CG2	2.48	0.43
1:B:264:PHE:CD1	1:B:264:PHE:C	2.92	0.43
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.92	0.43
1:F:208:LYS:O	1:F:275:PHE:HA	2.18	0.43
1:H:208:LYS:O	1:H:275:PHE:HA	2.19	0.43
1:A:280:LEU:O	1:A:284:ARG:HG2	2.19	0.43
1:B:33:LEU:HA	1:B:33:LEU:HD12	1.85	0.43
1:B:45:LEU:HD21	1:B:174:ARG:NH2	2.33	0.43
1:F:184:VAL:HG21	1:F:243:PHE:CE2	2.54	0.43
1:G:105:LEU:HD12	1:G:105:LEU:HA	1.90	0.43
1:I:116:SER:HB2	2:I:2408:NAP:H6N	2.00	0.43
1:A:208:LYS:HA	1:A:241:GLU:O	2.19	0.43
1:C:284:ARG:HD2	1:C:288:TYR:O	2.19	0.43
1:F:193:ASN:HB2	4:F:1309:HOH:O	2.18	0.43
1:B:116:SER:HB2	2:B:2401:NAP:H6N	2.01	0.42
1:F:22:LYS:HE2	1:F:226:GLU:OE2	2.19	0.42
1:I:247:ALA:HB1	1:I:259:ILE:HD11	2.00	0.42
1:J:260:GLU:O	1:J:260:GLU:HG3	2.19	0.42
1:I:179:GLY:O	1:I:187:HIS:HE1	2.02	0.42
1:B:5:THR:OG1	1:B:74:HIS:HA	2.19	0.42
1:C:105:LEU:HD11	1:C:162:ILE:HD11	2.01	0.42
1:D:192:LEU:HD11	1:D:251:LEU:CD2	2.50	0.42
1:G:127:PHE:CZ	1:G:276:THR:HA	2.54	0.42
1:I:84:TRP:CE3	1:I:139:VAL:HG22	2.55	0.42
1:A:294:THR:OG1	1:A:297:GLU:HG3	2.19	0.42
1:G:170:VAL:CG1	1:G:214:VAL:HG13	2.49	0.42
1:G:170:VAL:HG12	1:G:214:VAL:HG13	2.01	0.42
1:G:239:ARG:NH2	1:G:294:THR:HA	2.34	0.42
1:I:237:THR:HB	1:I:239:ARG:NH2	2.34	0.42
1:A:179:GLY:O	1:A:187:HIS:HE1	2.03	0.42
1:F:170:VAL:CG1	1:F:214:VAL:HG13	2.49	0.42
1:J:79:SER:HA	1:J:140:TYR:CE1	2.55	0.42
1:J:200:LEU:O	1:J:261:TYR:HA	2.20	0.42
1:A:240:ALA:N	1:A:277:GLN:HE21	2.18	0.42
1:D:40:VAL:HA	1:D:43:VAL:HG22	2.02	0.42
1:G:105:LEU:HD21	1:G:154:ILE:HG21	2.02	0.42
1:H:184:VAL:HG21	1:H:243:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:SER:OG	1:I:244:GLN:HB2	2.19	0.42
1:B:79:SER:HA	1:B:140:TYR:CE1	2.55	0.42
1:D:184:VAL:O	1:D:188:LEU:HG	2.20	0.42
1:E:194:ASN:C	1:E:196:GLU:H	2.23	0.42
1:E:79:SER:HB2	4:E:1489:HOH:O	2.19	0.42
1:I:171:TYR:OH	1:I:298:GLY:HA3	2.19	0.42
1:A:172:GLY:HA3	1:A:214:VAL:CG2	2.49	0.41
1:D:262:ILE:HG23	1:D:263:PRO:HD2	2.02	0.41
1:E:237:THR:HG22	1:E:292:PHE:HB3	2.02	0.41
1:G:239:ARG:HH21	1:G:294:THR:HA	1.85	0.41
1:D:121:GLY:HA3	1:D:135:LYS:O	2.20	0.41
1:G:134:GLU:OE1	1:G:152:ARG:NH2	2.53	0.41
1:H:116:SER:HB2	2:H:2407:NAP:H6N	2.02	0.41
1:A:241:GLU:OE1	1:A:295:VAL:HB	2.20	0.41
1:E:57:LEU:HD11	1:E:99:GLU:HG2	2.02	0.41
1:F:240:ALA:N	1:F:277:GLN:HE21	2.14	0.41
1:H:95:GLN:NE2	1:H:98:LYS:HE2	2.35	0.41
1:J:199:LYS:HA	1:J:260:GLU:O	2.20	0.41
1:A:209:ARG:HG3	1:A:276:THR:OG1	2.21	0.41
1:D:127:PHE:CZ	1:D:276:THR:HA	2.55	0.41
1:D:84:TRP:CH2	1:D:138:ASN:HA	2.55	0.41
3:E:2504:ADQ:H8	3:E:2504:ADQ:H5'2	2.00	0.41
1:F:116:SER:HB2	2:F:2405:NAP:H6N	2.02	0.41
1:G:93:ASN:N	1:G:93:ASN:HD22	2.17	0.41
1:C:166:ARG:HB2	1:C:234:ASN:HA	2.02	0.41
1:I:102:HIS:CE1	1:I:150:TYR:OH	2.73	0.41
1:J:17:LYS:HE2	4:J:906:HOH:O	2.20	0.41
1:B:299:VAL:O	1:B:303:MET:HG2	2.21	0.41
1:H:240:ALA:N	1:H:277:GLN:HE21	2.11	0.41
1:J:146:LEU:HD12	1:J:146:LEU:HA	1.93	0.41
1:D:134:GLU:CD	1:D:152:ARG:HH22	2.22	0.41
1:E:198:PRO:HD2	1:E:258:GLN:O	2.21	0.41
1:E:299:VAL:O	1:E:303:MET:HG2	2.20	0.41
1:G:205:GLU:HA	1:G:205:GLU:OE1	2.19	0.41
1:B:102:HIS:HE1	1:B:150:TYR:OH	2.03	0.41
1:C:79:SER:HA	1:C:140:TYR:CE1	2.56	0.41
1:A:127:PHE:CZ	1:A:276:THR:HA	2.56	0.41
1:A:209:ARG:NH1	1:A:243:PHE:HZ	2.19	0.41
1:E:105:LEU:HA	1:E:105:LEU:HD12	1.93	0.41
1:F:17:LYS:HD3	1:F:45:LEU:HD21	2.01	0.41
1:D:239:ARG:HB2	1:D:239:ARG:HE	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:HA	1:E:198:PRO:HD3	1.73	0.41
1:G:146:LEU:HA	1:G:146:LEU:HD12	1.89	0.41
1:C:241:GLU:OE1	1:C:295:VAL:HB	2.21	0.41
1:E:263:PRO:O	1:E:264:PHE:CB	2.64	0.41
1:E:264:PHE:HD2	1:E:264:PHE:HA	1.68	0.41
1:G:55:ASP:O	1:G:59:GLN:HG3	2.21	0.41
1:B:37:THR:O	1:B:40:VAL:HG22	2.21	0.40
1:G:10:PHE:CE1	1:G:214:VAL:HG11	2.56	0.40
1:H:33:LEU:HA	1:H:33:LEU:HD12	1.96	0.40
1:C:169:ASN:HD21	1:C:209:ARG:NH1	2.08	0.40
1:J:113:TYR:HB2	4:J:1127:HOH:O	2.21	0.40
1:J:1:MET:O	1:J:70:GLU:HG2	2.21	0.40
1:F:102:HIS:HE1	1:F:150:TYR:OH	2.04	0.40
1:G:132:GLU:CD	1:G:132:GLU:H	2.24	0.40
1:G:239:ARG:HA	1:G:277:GLN:NE2	2.37	0.40
1:I:264:PHE:HA	1:I:265:PRO:HD3	1.89	0.40
1:J:94:TYR:CZ	1:J:98:LYS:HD3	2.56	0.40
1:A:39:PHE:CE1	1:A:43:VAL:CG1	3.05	0.40
1:G:10:PHE:CZ	1:G:214:VAL:HG13	2.57	0.40
1:G:170:VAL:HA	1:G:212:VAL:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	266/310 (86%)	254 (96%)	9 (3%)	3 (1%)	17 9
1	B	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	44 40
1	C	265/310 (86%)	251 (95%)	13 (5%)	1 (0%)	38 33
1	D	304/310 (98%)	292 (96%)	11 (4%)	1 (0%)	44 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	44	40
1	F	304/310 (98%)	290 (95%)	13 (4%)	1 (0%)	44	40
1	G	304/310 (98%)	291 (96%)	11 (4%)	2 (1%)	25	18
1	H	292/310 (94%)	282 (97%)	10 (3%)	0	100	100
1	I	304/310 (98%)	290 (95%)	14 (5%)	0	100	100
1	J	295/310 (95%)	280 (95%)	12 (4%)	3 (1%)	18	10
All	All	2924/3100 (94%)	2798 (96%)	113 (4%)	13 (0%)	38	33

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	B	263	PRO
1	F	264	PHE
1	J	263	PRO
1	J	259	ILE
1	A	306	LEU
1	G	10	PHE
1	G	204	SER
1	D	10	PHE
1	A	10	PHE
1	E	10	PHE
1	J	199	LYS
1	C	122	GLY

### 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	222/256 (87%)	205 (92%)	17 (8%)	15	9
1	B	248/256 (97%)	226 (91%)	22 (9%)	11	7
1	C	224/256 (88%)	208 (93%)	16 (7%)	17	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	254/256 (99%)	235 (92%)	19 (8%)	16	10
1	E	248/256 (97%)	230 (93%)	18 (7%)	16	11
1	F	254/256 (99%)	235 (92%)	19 (8%)	16	10
1	G	254/256 (99%)	238 (94%)	16 (6%)	21	15
1	H	245/256 (96%)	227 (93%)	18 (7%)	16	11
1	I	254/256 (99%)	234 (92%)	20 (8%)	14	9
1	J	248/256 (97%)	229 (92%)	19 (8%)	15	9
All	All	2451/2560 (96%)	2267 (92%)	184 (8%)	16	10

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	43	VAL
1	A	91	ASP
1	A	105	LEU
1	A	124	THR
1	A	130	SER
1	A	131	ARG
1	A	138	ASN
1	A	139	VAL
1	A	157	GLU
1	A	209	ARG
1	A	212	VAL
1	A	214	VAL
1	A	226	GLU
1	A	250	THR
1	A	283	LEU
1	A	300	THR
1	B	1	MET
1	B	33	LEU
1	B	43	VAL
1	B	68	ASP
1	B	79	SER
1	B	91	ASP
1	B	99	GLU
1	B	105	LEU
1	B	124	THR
1	B	130	SER
1	B	131	ARG

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	139	VAL
1	B	157	GLU
1	B	174	ARG
1	B	204	SER
1	B	212	VAL
1	B	214	VAL
1	B	263	PRO
1	B	264	PHE
1	B	283	LEU
1	B	300	THR
1	C	1	MET
1	C	43	VAL
1	C	64	GLU
1	C	91	ASP
1	C	100	LEU
1	C	105	LEU
1	C	124	THR
1	C	130	SER
1	C	131	ARG
1	C	138	ASN
1	C	139	VAL
1	C	157	GLU
1	C	160	SER
1	C	212	VAL
1	C	214	VAL
1	C	283	LEU
1	D	43	VAL
1	D	91	ASP
1	D	99	GLU
1	D	105	LEU
1	D	124	THR
1	D	130	SER
1	D	131	ARG
1	D	138	ASN
1	D	139	VAL
1	D	157	GLU
1	D	160	SER
1	D	190	THR
1	D	205	GLU
1	D	212	VAL
1	D	214	VAL

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Mol	Chain	Res	Type
1	D	239	ARG
1	D	250	THR
1	D	283	LEU
1	D	300	THR
1	E	43	VAL
1	E	70	GLU
1	E	79	SER
1	E	91	ASP
1	E	99	GLU
1	E	105	LEU
1	E	124	THR
1	E	131	ARG
1	E	138	ASN
1	E	139	VAL
1	E	157	GLU
1	E	181	MET
1	E	212	VAL
1	E	214	VAL
1	E	256	LYS
1	E	264	PHE
1	E	272	TYR
1	E	283	LEU
1	F	43	VAL
1	F	79	SER
1	F	91	ASP
1	F	99	GLU
1	F	105	LEU
1	F	124	THR
1	F	131	ARG
1	F	132	GLU
1	F	138	ASN
1	F	139	VAL
1	F	157	GLU
1	F	160	SER
1	F	212	VAL
1	F	214	VAL
1	F	266	ASP
1	F	269	LYS
1	F	271	ARG
1	F	283	LEU
1	F	300	THR
1	G	33	LEU

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Mol	Chain	Res	Type
1	G	70	GLU
1	G	91	ASP
1	G	99	GLU
1	G	105	LEU
1	G	124	THR
1	G	131	ARG
1	G	132	GLU
1	G	138	ASN
1	G	139	VAL
1	G	157	GLU
1	G	160	SER
1	G	212	VAL
1	G	214	VAL
1	G	283	LEU
1	G	300	THR
1	H	1	MET
1	H	33	LEU
1	H	43	VAL
1	H	54	GLU
1	H	79	SER
1	H	91	ASP
1	H	99	GLU
1	H	105	LEU
1	H	130	SER
1	H	131	ARG
1	H	138	ASN
1	H	139	VAL
1	H	157	GLU
1	H	194	ASN
1	H	212	VAL
1	H	214	VAL
1	H	283	LEU
1	H	300	THR
1	I	1	MET
1	I	43	VAL
1	I	70	GLU
1	I	91	ASP
1	I	105	LEU
1	I	124	THR
1	I	130	SER
1	I	131	ARG
1	I	138	ASN

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Mol	Chain	Res	Type
1	I	139	VAL
1	I	156	PRO
1	I	157	GLU
1	I	160	SER
1	I	202	GLU
1	I	212	VAL
1	I	214	VAL
1	I	244	GLN
1	I	260	GLU
1	I	283	LEU
1	I	300	THR
1	J	68	ASP
1	J	79	SER
1	J	91	ASP
1	J	105	LEU
1	J	106	GLU
1	J	124	THR
1	J	126	ASP
1	J	130	SER
1	J	131	ARG
1	J	138	ASN
1	J	139	VAL
1	J	156	PRO
1	J	157	GLU
1	J	191	GLN
1	J	198	PRO
1	J	212	VAL
1	J	214	VAL
1	J	244	GLN
1	J	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	95	GLN
1	A	102	HIS
1	A	138	ASN
1	A	277	GLN
1	A	282	ASN
1	B	93	ASN
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	102	HIS
1	B	138	ASN
1	B	187	HIS
1	B	254	HIS
1	B	277	GLN
1	B	282	ASN
1	C	93	ASN
1	C	95	GLN
1	C	102	HIS
1	C	138	ASN
1	C	169	ASN
1	C	187	HIS
1	C	277	GLN
1	C	282	ASN
1	D	93	ASN
1	D	95	GLN
1	D	102	HIS
1	D	138	ASN
1	D	187	HIS
1	D	206	ASN
1	D	227	ASN
1	D	254	HIS
1	D	258	GLN
1	D	277	GLN
1	D	282	ASN
1	E	93	ASN
1	E	95	GLN
1	E	102	HIS
1	E	138	ASN
1	E	169	ASN
1	E	187	HIS
1	E	277	GLN
1	E	282	ASN
1	F	93	ASN
1	F	95	GLN
1	F	102	HIS
1	F	138	ASN
1	F	169	ASN
1	F	187	HIS
1	F	254	HIS
1	F	277	GLN
1	G	93	ASN

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Mol	Chain	Res	Type
1	G	95	GLN
1	G	102	HIS
1	G	138	ASN
1	G	169	ASN
1	G	187	HIS
1	G	254	HIS
1	G	273	GLN
1	G	277	GLN
1	G	282	ASN
1	H	93	ASN
1	H	95	GLN
1	H	102	HIS
1	H	138	ASN
1	H	169	ASN
1	H	187	HIS
1	H	189	ASN
1	H	194	ASN
1	H	254	HIS
1	H	277	GLN
1	H	282	ASN
1	I	93	ASN
1	I	95	GLN
1	I	102	HIS
1	I	138	ASN
1	I	169	ASN
1	I	187	HIS
1	I	254	HIS
1	I	258	GLN
1	I	273	GLN
1	I	277	GLN
1	I	282	ASN
1	J	93	ASN
1	J	95	GLN
1	J	102	HIS
1	J	138	ASN
1	J	169	ASN
1	J	187	HIS
1	J	189	ASN
1	J	227	ASN
1	J	254	HIS
1	J	273	GLN
1	J	277	GLN

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Mol	Chain	Res	Type
1	J	282	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSO	A	78	1	4,6,7	1.42	1 (25%)	1,6,8	1.73	0
1	CSO	B	78	1	4,6,7	1.48	1 (25%)	1,6,8	1.68	0
1	CSO	C	78	1	4,6,7	1.78	1 (25%)	1,6,8	1.71	0
1	CSO	D	78	1	4,6,7	1.88	1 (25%)	1,6,8	1.63	0
1	CSO	E	78	1	4,6,7	1.65	1 (25%)	1,6,8	1.64	0
1	CSO	F	78	1	4,6,7	0.96	0	1,6,8	1.78	0
1	CSO	G	78	1	4,6,7	1.66	1 (25%)	1,6,8	1.51	0
1	CSO	H	78	1	4,6,7	1.75	1 (25%)	1,6,8	1.95	0
1	CSO	I	78	1	4,6,7	1.78	1 (25%)	1,6,8	1.44	0
1	CSO	J	78	1	4,6,7	1.80	1 (25%)	1,6,8	1.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	78	1	-	0/1/5/7	0/0/0/0
1	CSO	B	78	1	-	0/1/5/7	0/0/0/0
1	CSO	C	78	1	-	0/1/5/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	D	78	1	-	0/1/5/7	0/0/0/0
1	CSO	E	78	1	-	0/1/5/7	0/0/0/0
1	CSO	F	78	1	-	0/1/5/7	0/0/0/0
1	CSO	G	78	1	-	0/1/5/7	0/0/0/0
1	CSO	H	78	1	-	0/1/5/7	0/0/0/0
1	CSO	I	78	1	-	0/1/5/7	0/0/0/0
1	CSO	J	78	1	-	0/1/5/7	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CSO	CA-C	2.68	1.53	1.50
1	B	78	CSO	CA-C	2.83	1.54	1.50
1	E	78	CSO	CA-C	3.02	1.54	1.50
1	G	78	CSO	CA-C	3.09	1.54	1.50
1	H	78	CSO	CA-C	3.34	1.54	1.50
1	C	78	CSO	CA-C	3.35	1.54	1.50
1	I	78	CSO	CA-C	3.38	1.54	1.50
1	J	78	CSO	CA-C	3.44	1.54	1.50
1	D	78	CSO	CA-C	3.55	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	78	CSO	1	0
1	B	78	CSO	1	0
1	C	78	CSO	1	0
1	D	78	CSO	1	0
1	E	78	CSO	1	0
1	F	78	CSO	1	0
1	G	78	CSO	1	0
1	H	78	CSO	1	0
1	I	78	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

20 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	NAP	A	2400	-	44,52,52	2.15	10 (22%)	51,80,80	1.95	9 (17%)
3	ADQ	A	2500	-	25,29,41	1.29	4 (16%)	24,45,63	2.37	3 (12%)
2	NAP	B	2401	-	44,52,52	2.08	8 (18%)	51,80,80	2.01	7 (13%)
3	ADQ	B	2501	-	35,41,41	1.38	4 (11%)	42,63,63	2.28	8 (19%)
2	NAP	C	2402	-	44,52,52	2.00	8 (18%)	51,80,80	2.01	7 (13%)
3	ADQ	C	2502	-	25,29,41	1.04	2 (8%)	24,45,63	2.36	2 (8%)
2	NAP	D	2403	-	44,52,52	2.05	10 (22%)	51,80,80	1.88	7 (13%)
3	ADQ	D	2503	-	35,41,41	1.52	4 (11%)	42,63,63	2.50	8 (19%)
2	NAP	E	2404	-	44,52,52	2.17	10 (22%)	51,80,80	1.96	10 (19%)
3	ADQ	E	2504	-	25,29,41	1.20	4 (16%)	24,45,63	2.40	3 (12%)
2	NAP	F	2405	-	44,52,52	2.06	10 (22%)	51,80,80	2.01	10 (19%)
3	ADQ	F	2505	-	35,41,41	1.49	6 (17%)	42,63,63	2.33	8 (19%)
2	NAP	G	2406	-	44,52,52	2.03	10 (22%)	51,80,80	1.97	10 (19%)
3	ADQ	G	2506	-	25,29,41	1.34	3 (12%)	24,45,63	2.29	2 (8%)
2	NAP	H	2407	-	44,52,52	2.10	7 (15%)	51,80,80	1.99	8 (15%)
3	ADQ	H	2507	-	25,29,41	1.27	3 (12%)	24,45,63	2.35	2 (8%)
2	NAP	I	2408	-	44,52,52	2.05	9 (20%)	51,80,80	1.96	9 (17%)
3	ADQ	I	2508	-	25,29,41	1.08	2 (8%)	24,45,63	2.32	3 (12%)
2	NAP	J	2409	-	44,52,52	2.24	10 (22%)	51,80,80	1.98	7 (13%)
3	ADQ	J	2509	-	25,29,41	1.19	4 (16%)	24,45,63	2.46	3 (12%)

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	NAP	A	2400	-	-	0/27/67/67	0/5/5/5
3	ADQ	A	2500	-	-	0/12/32/59	0/3/3/4
2	NAP	B	2401	-	-	0/27/67/67	0/5/5/5
3	ADQ	B	2501	-	-	0/19/59/59	0/4/4/4
2	NAP	C	2402	-	-	0/27/67/67	0/5/5/5
3	ADQ	C	2502	-	-	0/12/32/59	0/3/3/4
2	NAP	D	2403	-	-	0/27/67/67	0/5/5/5
3	ADQ	D	2503	-	-	0/19/59/59	0/4/4/4
2	NAP	E	2404	-	-	0/27/67/67	0/5/5/5
3	ADQ	E	2504	-	-	0/12/32/59	0/3/3/4
2	NAP	F	2405	-	-	0/27/67/67	0/5/5/5
3	ADQ	F	2505	-	-	0/19/59/59	0/4/4/4
2	NAP	G	2406	-	1/1/12/12	0/27/67/67	0/5/5/5
3	ADQ	G	2506	-	-	0/12/32/59	0/3/3/4
2	NAP	H	2407	-	-	0/27/67/67	0/5/5/5
3	ADQ	H	2507	-	-	0/12/32/59	0/3/3/4
2	NAP	I	2408	-	-	0/27/67/67	0/5/5/5
3	ADQ	I	2508	-	-	0/12/32/59	0/3/3/4
2	NAP	J	2409	-	-	0/27/67/67	0/5/5/5
3	ADQ	J	2509	-	-	0/12/32/59	0/3/3/4

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2503	ADQ	PB-O3B	-5.46	1.47	1.60
3	F	2505	ADQ	PB-O3B	-4.47	1.49	1.60
3	B	2501	ADQ	PB-O3B	-3.98	1.50	1.60
3	I	2508	ADQ	PB-O3A	-2.95	1.55	1.60
3	E	2504	ADQ	PB-O3A	-2.85	1.55	1.60
3	A	2500	ADQ	PB-O3A	-2.70	1.55	1.60
3	G	2506	ADQ	PB-O3A	-2.57	1.55	1.60
3	E	2504	ADQ	C5-N7	-2.55	1.30	1.39
2	D	2403	NAP	P2B-O3X	-2.44	1.44	1.54
3	A	2500	ADQ	C5-N7	-2.31	1.31	1.39
2	I	2408	NAP	P2B-O3X	-2.31	1.45	1.54
2	G	2406	NAP	P2B-O3X	-2.25	1.45	1.54
3	J	2509	ADQ	PB-O3A	-2.22	1.56	1.60
3	B	2501	ADQ	C5-N7	-2.22	1.31	1.39
2	A	2400	NAP	P2B-O3X	-2.22	1.45	1.54
2	C	2402	NAP	P2B-O3X	-2.19	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2404	NAP	P2B-O3X	-2.17	1.45	1.54
3	J	2509	ADQ	C5-N7	-2.14	1.32	1.39
3	F	2505	ADQ	C5-N7	-2.13	1.32	1.39
3	H	2507	ADQ	C5-N7	-2.12	1.32	1.39
2	F	2405	NAP	P2B-O3X	-2.08	1.46	1.54
2	J	2409	NAP	P2B-O3X	-2.05	1.46	1.54
2	E	2404	NAP	O4B-C1B	2.01	1.44	1.41
2	D	2403	NAP	C6N-N1N	2.06	1.40	1.35
2	E	2404	NAP	C6N-N1N	2.07	1.40	1.35
2	F	2405	NAP	C2N-C3N	2.07	1.42	1.39
3	G	2506	ADQ	PB-O2B	2.07	1.63	1.54
2	D	2403	NAP	O4B-C1B	2.08	1.44	1.41
2	B	2401	NAP	C5B-C4B	2.09	1.58	1.51
2	A	2400	NAP	O4D-C1D	2.09	1.44	1.41
3	C	2502	ADQ	O4D-C1D	2.10	1.44	1.41
3	I	2508	ADQ	PB-O2B	2.12	1.63	1.54
2	F	2405	NAP	O4B-C1B	2.13	1.44	1.41
2	J	2409	NAP	C6N-N1N	2.13	1.41	1.35
2	G	2406	NAP	C3B-C2B	2.13	1.57	1.53
2	G	2406	NAP	O4D-C1D	2.14	1.44	1.41
3	F	2505	ADQ	C4'-C3'	2.15	1.57	1.52
3	B	2501	ADQ	C3'-C2'	2.17	1.57	1.52
2	J	2409	NAP	O4B-C1B	2.21	1.44	1.41
3	J	2509	ADQ	PB-O2B	2.22	1.63	1.54
3	F	2505	ADQ	O2'-C2'	2.23	1.48	1.43
3	D	2503	ADQ	O2'-C2'	2.23	1.48	1.43
2	A	2400	NAP	C5B-C4B	2.25	1.58	1.51
3	F	2505	ADQ	O4D-C1D	2.25	1.44	1.41
3	E	2504	ADQ	C2-N3	2.35	1.36	1.32
2	E	2404	NAP	C2A-N1A	2.38	1.38	1.33
2	H	2407	NAP	C5N-C4N	2.39	1.43	1.38
2	C	2402	NAP	C5N-C4N	2.40	1.43	1.38
3	B	2501	ADQ	O4D-C1D	2.40	1.44	1.41
3	E	2504	ADQ	O4D-C1D	2.44	1.44	1.41
2	I	2408	NAP	C6N-N1N	2.44	1.41	1.35
2	B	2401	NAP	C5N-C4N	2.48	1.43	1.38
3	A	2500	ADQ	PB-O2B	2.48	1.65	1.54
2	C	2402	NAP	C7N-N7N	2.50	1.37	1.33
2	I	2408	NAP	C2A-N1A	2.54	1.38	1.33
3	D	2503	ADQ	C4'-C5'	2.54	1.58	1.53
2	F	2405	NAP	C2A-N1A	2.57	1.38	1.33
3	C	2502	ADQ	PB-O2B	2.59	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2507	ADQ	PB-O2B	2.63	1.65	1.54
2	B	2401	NAP	C2A-N1A	2.64	1.38	1.33
2	B	2401	NAP	C3B-C2B	2.70	1.59	1.53
2	I	2408	NAP	C7N-N7N	2.75	1.38	1.33
2	G	2406	NAP	C7N-N7N	2.77	1.38	1.33
2	H	2407	NAP	C7N-N7N	2.83	1.38	1.33
2	A	2400	NAP	C2A-N1A	2.83	1.39	1.33
3	D	2503	ADQ	O4D-C1D	2.85	1.45	1.41
2	H	2407	NAP	C2A-N1A	2.86	1.39	1.33
2	D	2403	NAP	C7N-N7N	2.86	1.38	1.33
2	B	2401	NAP	C4N-C3N	2.87	1.44	1.39
2	C	2402	NAP	C3B-C2B	2.89	1.59	1.53
2	A	2400	NAP	C7N-N7N	2.90	1.38	1.33
2	J	2409	NAP	C7N-N7N	2.95	1.38	1.33
2	J	2409	NAP	C5N-C4N	2.95	1.44	1.38
2	I	2408	NAP	C5N-C4N	2.95	1.44	1.38
2	D	2403	NAP	C2A-N1A	2.96	1.39	1.33
2	E	2404	NAP	C7N-N7N	2.98	1.38	1.33
2	F	2405	NAP	C3B-C2B	2.99	1.59	1.53
2	D	2403	NAP	C5N-C4N	3.03	1.44	1.38
2	A	2400	NAP	C5N-C4N	3.05	1.44	1.38
3	A	2500	ADQ	O4D-C1D	3.08	1.45	1.41
2	F	2405	NAP	C7N-N7N	3.11	1.39	1.33
2	J	2409	NAP	C2A-N1A	3.12	1.39	1.33
2	G	2406	NAP	C2A-N1A	3.17	1.39	1.33
2	B	2401	NAP	C7N-N7N	3.18	1.39	1.33
2	C	2402	NAP	C4N-C3N	3.24	1.44	1.39
3	F	2505	ADQ	C3'-C2'	3.25	1.60	1.52
2	E	2404	NAP	C5N-C4N	3.26	1.45	1.38
2	C	2402	NAP	C2A-N1A	3.27	1.40	1.33
2	E	2404	NAP	C3B-C2B	3.28	1.60	1.53
2	F	2405	NAP	C5N-C4N	3.29	1.45	1.38
2	G	2406	NAP	C5N-C4N	3.30	1.45	1.38
2	I	2408	NAP	C3B-C2B	3.30	1.60	1.53
2	H	2407	NAP	C3B-C2B	3.33	1.60	1.53
3	J	2509	ADQ	O4D-C1D	3.37	1.45	1.41
2	D	2403	NAP	C3B-C2B	3.40	1.60	1.53
2	J	2409	NAP	C3B-C2B	3.50	1.60	1.53
2	D	2403	NAP	C4N-C3N	3.56	1.45	1.39
2	F	2405	NAP	C4N-C3N	3.59	1.45	1.39
2	H	2407	NAP	C4N-C3N	3.59	1.45	1.39
2	A	2400	NAP	C3B-C2B	3.72	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2400	NAP	C4N-C3N	3.74	1.45	1.39
2	G	2406	NAP	C4N-C3N	3.84	1.45	1.39
2	I	2408	NAP	C4N-C3N	3.87	1.45	1.39
3	H	2507	ADQ	O4D-C1D	3.93	1.46	1.41
2	G	2406	NAP	O4B-C1B	4.00	1.46	1.41
3	G	2506	ADQ	O4D-C1D	4.32	1.47	1.41
2	J	2409	NAP	C4N-C3N	4.33	1.46	1.39
2	E	2404	NAP	C4N-C3N	4.47	1.46	1.39
2	B	2401	NAP	C3N-C7N	4.71	1.57	1.50
2	H	2407	NAP	C3N-C7N	4.71	1.57	1.50
2	C	2402	NAP	C3N-C7N	4.76	1.57	1.50
2	F	2405	NAP	C3N-C7N	5.18	1.58	1.50
2	I	2408	NAP	C3N-C7N	5.33	1.58	1.50
2	D	2403	NAP	C3N-C7N	5.35	1.58	1.50
2	A	2400	NAP	C3N-C7N	5.67	1.59	1.50
2	E	2404	NAP	C3N-C7N	5.68	1.59	1.50
2	J	2409	NAP	C3N-C7N	6.02	1.59	1.50
2	G	2406	NAP	P2B-O2B	6.18	1.70	1.59
2	G	2406	NAP	C3N-C7N	6.78	1.61	1.50
2	D	2403	NAP	P2B-O2B	8.11	1.73	1.59
2	F	2405	NAP	P2B-O2B	8.34	1.74	1.59
2	C	2402	NAP	P2B-O2B	8.42	1.74	1.59
2	A	2400	NAP	P2B-O2B	8.47	1.74	1.59
2	I	2408	NAP	P2B-O2B	8.53	1.74	1.59
2	E	2404	NAP	P2B-O2B	8.72	1.74	1.59
2	H	2407	NAP	P2B-O2B	9.07	1.75	1.59
2	J	2409	NAP	P2B-O2B	9.28	1.75	1.59
2	B	2401	NAP	P2B-O2B	9.34	1.75	1.59

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2509	ADQ	N3-C2-N1	-11.09	119.20	128.86
3	F	2505	ADQ	N3-C2-N1	-11.01	119.27	128.86
3	E	2504	ADQ	N3-C2-N1	-10.89	119.38	128.86
3	B	2501	ADQ	N3-C2-N1	-10.77	119.47	128.86
3	D	2503	ADQ	N3-C2-N1	-10.77	119.48	128.86
3	A	2500	ADQ	N3-C2-N1	-10.77	119.48	128.86
3	H	2507	ADQ	N3-C2-N1	-10.74	119.50	128.86
3	C	2502	ADQ	N3-C2-N1	-10.71	119.53	128.86
3	G	2506	ADQ	N3-C2-N1	-10.61	119.62	128.86
3	I	2508	ADQ	N3-C2-N1	-10.31	119.88	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	C5N-C4N-C3N	-7.62	111.39	120.35
2	J	2409	NAP	C5N-C4N-C3N	-7.52	111.50	120.35
2	E	2404	NAP	C5N-C4N-C3N	-7.48	111.55	120.35
2	B	2401	NAP	C5N-C4N-C3N	-7.47	111.56	120.35
2	H	2407	NAP	C5N-C4N-C3N	-7.41	111.63	120.35
2	C	2402	NAP	C5N-C4N-C3N	-7.37	111.68	120.35
2	A	2400	NAP	C5N-C4N-C3N	-7.37	111.68	120.35
2	I	2408	NAP	C5N-C4N-C3N	-7.20	111.88	120.35
2	G	2406	NAP	C5N-C4N-C3N	-7.07	112.03	120.35
2	D	2403	NAP	C5N-C4N-C3N	-6.94	112.19	120.35
2	C	2402	NAP	C3N-C2N-N1N	-4.45	115.94	120.43
2	H	2407	NAP	C3N-C2N-N1N	-4.44	115.96	120.43
2	B	2401	NAP	C3N-C2N-N1N	-4.26	116.14	120.43
2	F	2405	NAP	C3N-C2N-N1N	-4.00	116.40	120.43
2	D	2403	NAP	C3N-C2N-N1N	-3.93	116.47	120.43
2	I	2408	NAP	C3N-C2N-N1N	-3.92	116.48	120.43
2	J	2409	NAP	C3N-C2N-N1N	-3.92	116.48	120.43
2	G	2406	NAP	C3N-C2N-N1N	-3.74	116.66	120.43
2	A	2400	NAP	C3N-C2N-N1N	-3.72	116.68	120.43
2	E	2404	NAP	C3N-C2N-N1N	-3.42	116.98	120.43
2	G	2406	NAP	C4B-O4B-C1B	-3.01	106.57	109.77
3	D	2503	ADQ	C4-C5-N7	-3.00	106.51	109.41
3	I	2508	ADQ	C4-C5-N7	-2.86	106.64	109.41
3	B	2501	ADQ	C4-C5-N7	-2.85	106.66	109.41
2	G	2406	NAP	C2B-C3B-C4B	-2.75	95.71	101.95
3	J	2509	ADQ	C4-C5-N7	-2.70	106.80	109.41
3	E	2504	ADQ	C4-C5-N7	-2.64	106.86	109.41
2	G	2406	NAP	O2B-P2B-O1X	-2.62	99.01	109.26
2	F	2405	NAP	O2B-P2B-O1X	-2.58	99.15	109.26
3	A	2500	ADQ	C4-C5-N7	-2.56	106.94	109.41
2	A	2400	NAP	O2B-P2B-O1X	-2.55	99.28	109.26
3	F	2505	ADQ	C4-C5-N7	-2.53	106.96	109.41
3	C	2502	ADQ	C4-C5-N7	-2.49	107.00	109.41
2	D	2403	NAP	O2B-P2B-O1X	-2.46	99.63	109.26
3	H	2507	ADQ	C4-C5-N7	-2.45	107.04	109.41
2	I	2408	NAP	O5B-C5B-C4B	-2.33	100.75	109.00
3	G	2506	ADQ	C4-C5-N7	-2.32	107.17	109.41
2	E	2404	NAP	C3B-C2B-C1B	-2.26	98.33	102.75
2	F	2405	NAP	C3B-C2B-C1B	-2.24	98.37	102.75
2	H	2407	NAP	O2B-P2B-O1X	-2.21	100.59	109.26
2	E	2404	NAP	O5B-C5B-C4B	-2.19	101.22	109.00
2	I	2408	NAP	O2B-P2B-O1X	-2.11	101.00	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	O5B-C5B-C4B	-2.09	101.58	109.00
2	J	2409	NAP	O2B-P2B-O1X	-2.04	101.28	109.26
2	A	2400	NAP	O3X-P2B-O2X	2.01	115.73	107.61
2	E	2404	NAP	O3X-P2B-O2X	2.01	115.73	107.61
3	I	2508	ADQ	C2D-C3D-C4D	2.02	106.56	102.62
2	I	2408	NAP	O3X-P2B-O2X	2.03	115.81	107.61
2	G	2406	NAP	O3X-P2B-O2X	2.04	115.84	107.61
2	E	2404	NAP	O7N-C7N-N7N	2.07	125.53	122.58
2	B	2401	NAP	O7N-C7N-N7N	2.11	125.59	122.58
3	F	2505	ADQ	O5'-C5'-C4'	2.12	113.56	109.66
2	C	2402	NAP	O3B-C3B-C2B	2.13	117.25	111.18
2	D	2403	NAP	N6A-C6A-N1A	2.14	123.00	118.77
2	A	2400	NAP	O7N-C7N-N7N	2.14	125.63	122.58
2	H	2407	NAP	O7N-C7N-N7N	2.21	125.72	122.58
2	H	2407	NAP	O3B-C3B-C2B	2.21	117.47	111.18
2	A	2400	NAP	N6A-C6A-N1A	2.22	123.18	118.77
2	F	2405	NAP	O7N-C7N-N7N	2.23	125.75	122.58
2	C	2402	NAP	N6A-C6A-N1A	2.26	123.24	118.77
3	A	2500	ADQ	C2D-C3D-C4D	2.28	107.06	102.62
3	E	2504	ADQ	C2D-C3D-C4D	2.29	107.08	102.62
2	F	2405	NAP	N6A-C6A-N1A	2.30	123.32	118.77
3	J	2509	ADQ	C2D-C3D-C4D	2.30	107.11	102.62
2	I	2408	NAP	N6A-C6A-N1A	2.32	123.36	118.77
2	E	2404	NAP	N6A-C6A-N1A	2.32	123.37	118.77
2	B	2401	NAP	N6A-C6A-N1A	2.32	123.37	118.77
2	J	2409	NAP	N6A-C6A-N1A	2.32	123.37	118.77
3	B	2501	ADQ	C1'-O5'-C5'	2.34	118.12	113.72
3	B	2501	ADQ	C2D-C3D-C4D	2.39	107.27	102.62
2	G	2406	NAP	N6A-C6A-N1A	2.39	123.51	118.77
3	F	2505	ADQ	C1'-O5'-C5'	2.44	118.31	113.72
3	B	2501	ADQ	O3B-C1'-C2'	2.46	112.89	108.38
3	F	2505	ADQ	O3B-C1'-C2'	2.52	112.99	108.38
3	D	2503	ADQ	O5'-C5'-C4'	2.66	114.55	109.66
2	G	2406	NAP	C4A-C5A-N7A	2.68	112.00	109.41
3	B	2501	ADQ	O5'-C5'-C4'	2.73	114.68	109.66
2	F	2405	NAP	C4A-C5A-N7A	2.73	112.05	109.41
2	C	2402	NAP	C4A-C5A-N7A	2.78	112.10	109.41
3	F	2505	ADQ	C1'-C2'-C3'	2.84	115.25	109.98
2	I	2408	NAP	C4A-C5A-N7A	2.88	112.19	109.41
2	D	2403	NAP	C4A-C5A-N7A	2.89	112.20	109.41
2	H	2407	NAP	C4A-C5A-N7A	2.90	112.21	109.41
2	J	2409	NAP	C4A-C5A-N7A	3.10	112.41	109.41

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2404	NAP	C4A-C5A-N7A	3.13	112.43	109.41
3	D	2503	ADQ	O4'-C4'-C3'	3.14	117.18	110.36
3	D	2503	ADQ	C1'-O5'-C5'	3.20	119.75	113.72
2	A	2400	NAP	C4A-C5A-N7A	3.22	112.53	109.41
3	F	2505	ADQ	O4'-C4'-C3'	3.32	117.59	110.36
2	B	2401	NAP	C4A-C5A-N7A	3.34	112.64	109.41
3	D	2503	ADQ	PB-O3B-C1'	3.42	133.30	119.74
3	B	2501	ADQ	O4'-C4'-C3'	3.75	118.53	110.36
2	E	2404	NAP	C6N-C5N-C4N	4.18	125.75	119.44
2	I	2408	NAP	C6N-C5N-C4N	4.44	126.13	119.44
2	D	2403	NAP	C6N-C5N-C4N	4.49	126.22	119.44
2	J	2409	NAP	C6N-C5N-C4N	4.58	126.34	119.44
2	G	2406	NAP	C6N-C5N-C4N	4.63	126.43	119.44
2	C	2402	NAP	C6N-C5N-C4N	4.74	126.58	119.44
2	H	2407	NAP	C6N-C5N-C4N	4.74	126.59	119.44
3	D	2503	ADQ	O3A-PB-O3B	4.75	110.54	102.05
2	A	2400	NAP	C6N-C5N-C4N	4.82	126.71	119.44
2	B	2401	NAP	C6N-C5N-C4N	4.86	126.77	119.44
2	F	2405	NAP	C6N-C5N-C4N	5.02	127.01	119.44
2	G	2406	NAP	C2N-C3N-C4N	5.71	124.77	118.26
3	B	2501	ADQ	O3A-PB-O3B	5.88	112.56	102.05
2	A	2400	NAP	C2N-C3N-C4N	5.94	125.04	118.26
2	D	2403	NAP	C2N-C3N-C4N	5.97	125.08	118.26
2	F	2405	NAP	C2N-C3N-C4N	6.09	125.21	118.26
2	E	2404	NAP	C2N-C3N-C4N	6.21	125.35	118.26
2	J	2409	NAP	C2N-C3N-C4N	6.22	125.36	118.26
3	F	2505	ADQ	O3A-PB-O3B	6.25	113.22	102.05
2	H	2407	NAP	C2N-C3N-C4N	6.36	125.52	118.26
2	I	2408	NAP	C2N-C3N-C4N	6.39	125.55	118.26
2	B	2401	NAP	C2N-C3N-C4N	6.40	125.57	118.26
2	C	2402	NAP	C2N-C3N-C4N	6.42	125.59	118.26
3	D	2503	ADQ	O3B-C1'-C2'	7.42	121.97	108.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	2406	NAP	C4B

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2400	NAP	1	0
3	A	2500	ADQ	3	0
2	B	2401	NAP	1	0
3	B	2501	ADQ	2	0
3	C	2502	ADQ	2	0
2	E	2404	NAP	1	0
3	E	2504	ADQ	3	0
2	F	2405	NAP	1	0
3	F	2505	ADQ	3	0
2	G	2406	NAP	1	0
2	H	2407	NAP	1	0
3	H	2507	ADQ	1	0
2	I	2408	NAP	1	0
3	I	2508	ADQ	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.