



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:01 PM GMT

PDB ID : 2D3C  
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with ADP and Phosphinothricin Phosphate  
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.  
Deposited on : 2005-09-26  
Resolution : 3.81 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

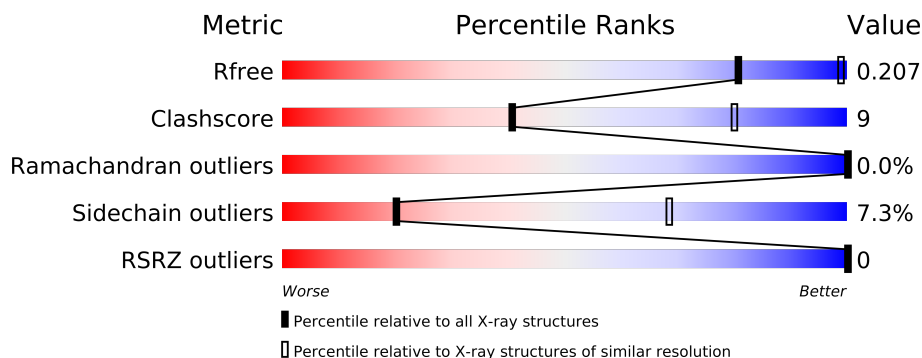
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.81 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	1165 (4.24-3.40)
Clashscore	79885	1105 (4.14-3.50)
Ramachandran outliers	78287	1055 (4.14-3.50)
Sidechain outliers	78261	1047 (4.14-3.50)
RSRZ outliers	66119	1166 (4.24-3.40)

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. 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	356	
1	B	356	
1	C	356	
1	D	356	
1	E	356	
1	F	356	
1	G	356	
1	H	356	
1	I	356	
1	J	356	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MN	F	1051	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28138 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

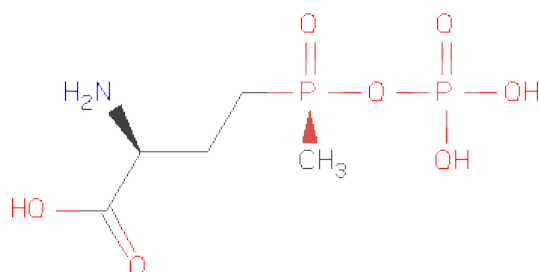
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mn	0	0
			3	3		
2	J	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		
2	E	3	Total	Mn	0	0
			3	3		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		
2	I	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		
2	A	3	Total	Mn	0	0
			3	3		
2	F	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (2S)-2-AMINO-4-[METHYL(PHOSPHONOOXY)PHOSPHORYL]BUTANOIC ACID (three-letter code: P3P) (formula:  $C_5H_{13}NO_7P_2$ ).



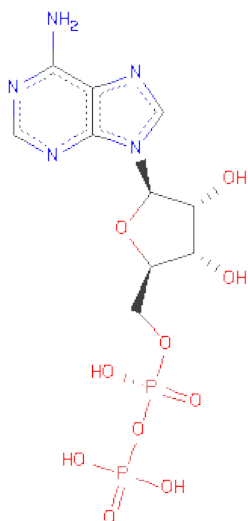
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	C	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	D	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	E	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	F	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	I	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	J	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	H	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

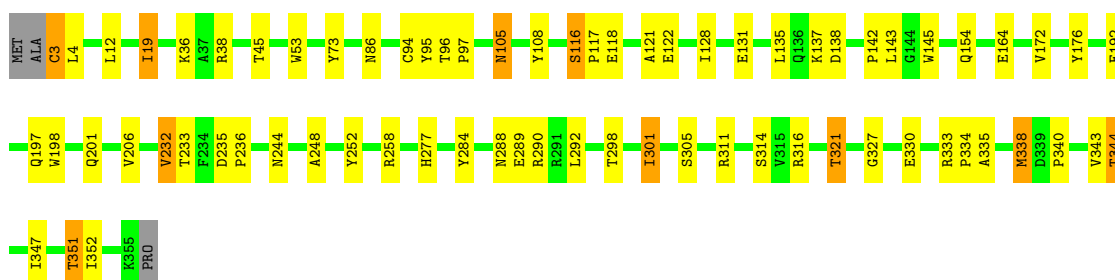
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	26	Total	O	0	0
			26	26		
5	C	11	Total	O	0	0
			11	11		
5	D	30	Total	O	0	0
			30	30		
5	E	30	Total	O	0	0
			30	30		
5	F	31	Total	O	0	0
			31	31		
5	G	22	Total	O	0	0
			22	22		
5	H	21	Total	O	0	0
			21	21		
5	I	27	Total	O	0	0
			27	27		
5	J	15	Total	O	0	0
			15	15		

### 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.

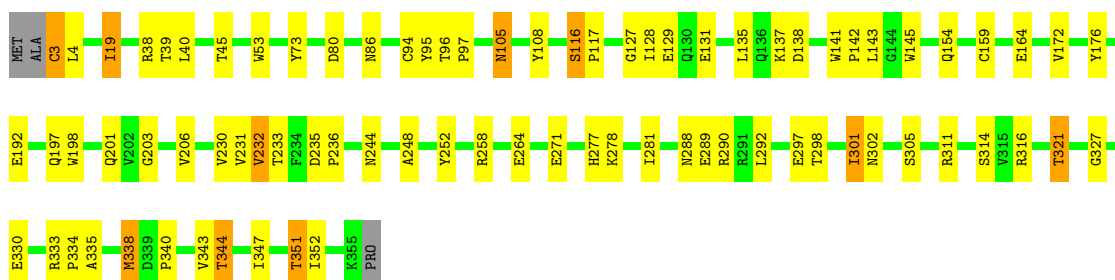
- Molecule 1: glutamine synthetase

Chain A:



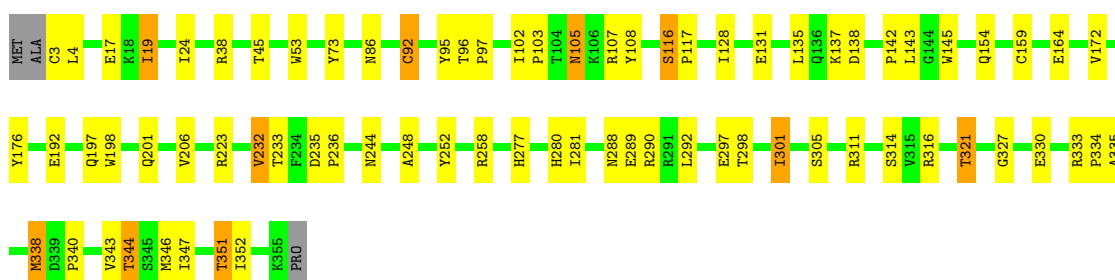
- Molecule 1: glutamine synthetase

Chain B:



- Molecule 1: glutamine synthetase

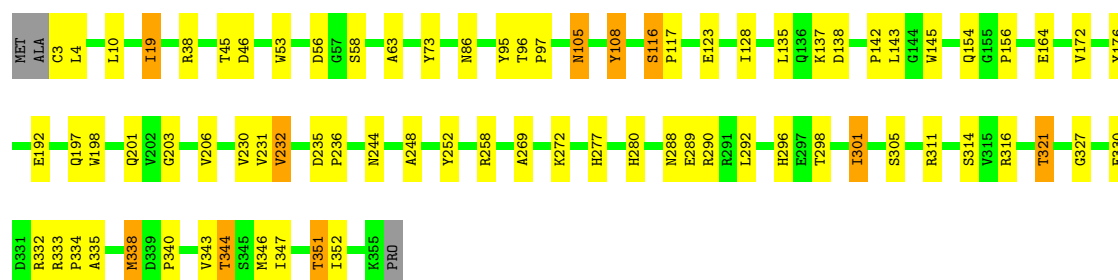
Chain C:



- Molecule 1: glutamine synthetase

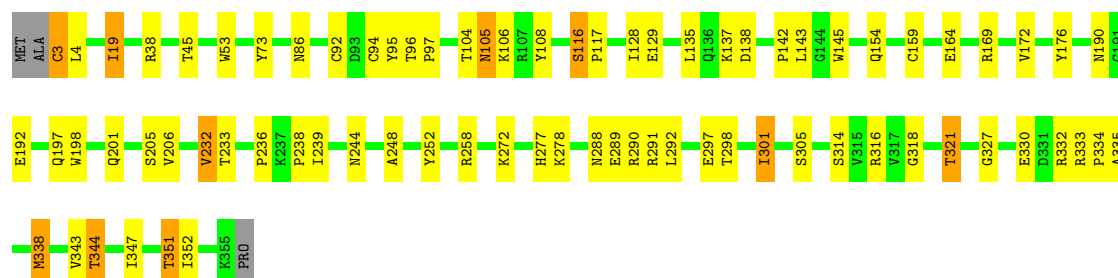
Chain D:





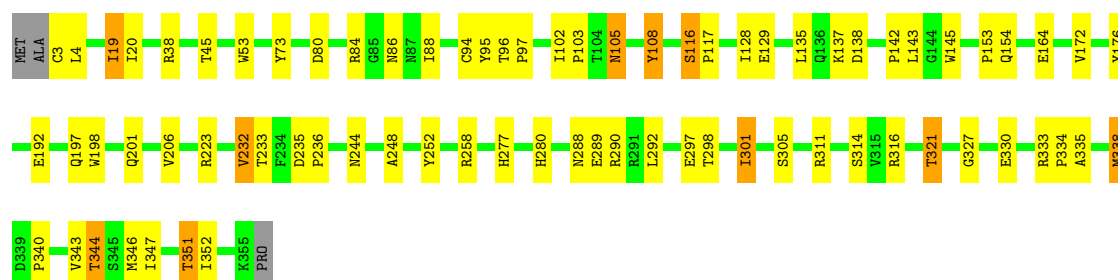
- Molecule 1: glutamine synthetase

Chain E:



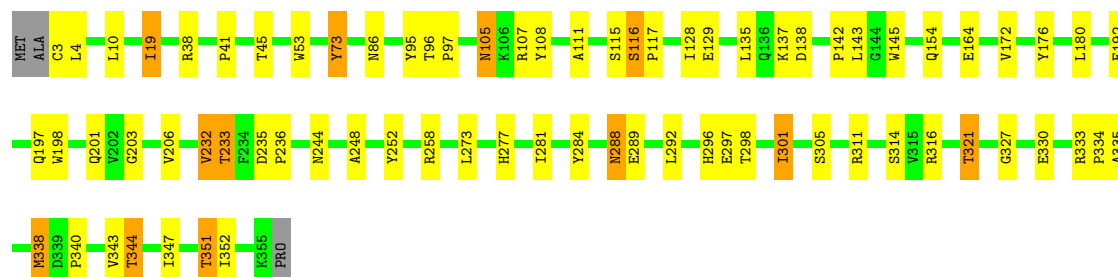
- Molecule 1: glutamine synthetase

Chain F:



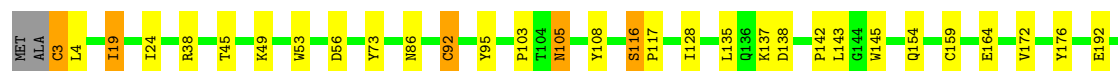
- Molecule 1: glutamine synthetase

Chain G:



- Molecule 1: glutamine synthetase

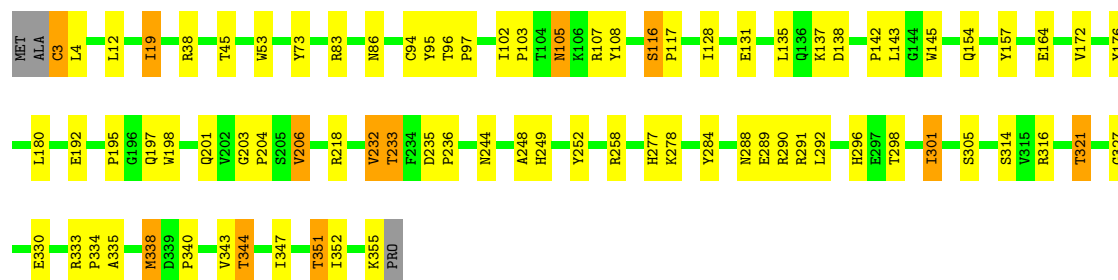
Chain H:





- Molecule 1: glutamine synthetase

Chain I:



- Molecule 1: glutamine synthetase

Chain J:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.96Å 191.01Å 118.12Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	27.36 – 3.81 27.36 – 3.81	Depositor EDS
% Data completeness (in resolution range)	83.0 (27.36-3.81) 83.1 (27.36-3.81)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.185 , 0.229 0.171 , 0.207	Depositor DCC
$R_{free}$ test set	1718 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 9.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 33883 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	28138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: P3P, MN, ADP

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	0.96	1/2819 (0.0%)	0.81	1/3834 (0.0%)
1	B	0.98	2/2819 (0.1%)	0.82	1/3834 (0.0%)
1	C	0.99	3/2819 (0.1%)	0.81	1/3834 (0.0%)
1	D	0.98	1/2819 (0.0%)	0.84	1/3834 (0.0%)
1	E	0.99	3/2819 (0.1%)	0.84	3/3834 (0.1%)
1	F	1.01	2/2819 (0.1%)	0.83	1/3834 (0.0%)
1	G	0.98	1/2819 (0.0%)	0.83	1/3834 (0.0%)
1	H	0.95	2/2819 (0.1%)	0.81	1/3834 (0.0%)
1	I	0.98	1/2819 (0.0%)	0.81	1/3834 (0.0%)
1	J	0.99	2/2819 (0.1%)	0.83	2/3834 (0.1%)
All	All	0.98	18/28190 (0.1%)	0.82	13/38340 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	94	CYS	CB-SG	-9.28	1.66	1.82
1	B	159	CYS	CB-SG	-8.08	1.68	1.82
1	A	94	CYS	CB-SG	-7.07	1.70	1.82
1	C	92	CYS	CB-SG	-6.33	1.71	1.82
1	J	94	CYS	CB-SG	-6.04	1.72	1.82
1	F	94	CYS	CB-SG	-5.57	1.72	1.81
1	J	17	GLU	CG-CD	5.52	1.60	1.51
1	E	94	CYS	CB-SG	-5.39	1.73	1.81
1	C	17	GLU	CG-CD	5.36	1.59	1.51
1	H	159	CYS	CB-SG	-5.30	1.73	1.81
1	C	159	CYS	CB-SG	-5.29	1.73	1.81
1	B	94	CYS	CB-SG	-5.21	1.73	1.81
1	E	159	CYS	CB-SG	-5.20	1.73	1.81
1	H	92	CYS	CB-SG	-5.19	1.73	1.81
1	D	108	TYR	CE2-CZ	5.11	1.45	1.38
1	G	73	TYR	CE2-CZ	5.07	1.45	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	92	CYS	CB-SG	-5.02	1.73	1.81
1	F	108	TYR	CE2-CZ	5.01	1.45	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	232	VAL	CB-CA-C	-5.50	100.95	111.40
1	F	232	VAL	CB-CA-C	-5.44	101.06	111.40
1	G	232	VAL	CB-CA-C	-5.39	101.15	111.40
1	E	232	VAL	CB-CA-C	-5.39	101.16	111.40
1	C	232	VAL	CB-CA-C	-5.25	101.43	111.40
1	B	232	VAL	CB-CA-C	-5.17	101.58	111.40
1	J	291	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	J	232	VAL	CB-CA-C	-5.09	101.72	111.40
1	A	232	VAL	CB-CA-C	-5.09	101.74	111.40
1	E	291	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	H	232	VAL	CB-CA-C	-5.03	101.85	111.40
1	I	232	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

There are no planarity outliers.

## 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	2745	0	2653	47	0
1	B	2745	0	2653	51	1
1	C	2745	0	2653	46	0
1	D	2745	0	2653	55	0
1	E	2745	0	2653	48	0
1	F	2745	0	2653	52	0
1	G	2745	0	2653	53	0
1	H	2745	0	2653	47	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2745	0	2653	56	0
1	J	2745	0	2653	44	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	15	0	10	5	0
3	B	15	0	10	3	0
3	C	15	0	10	4	0
3	D	15	0	10	3	0
3	E	15	0	10	4	0
3	F	15	0	10	4	0
3	G	15	0	10	2	0
3	H	15	0	10	2	0
3	I	15	0	10	4	0
3	J	15	0	10	0	0
4	A	27	0	12	0	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0
4	E	27	0	12	0	0
4	F	27	0	12	2	0
4	G	27	0	12	3	0
4	H	27	0	12	0	0
4	I	27	0	12	2	0
4	J	27	0	12	1	0
5	A	25	0	0	7	0
5	B	26	0	0	5	0
5	C	11	0	0	1	0
5	D	30	0	0	11	0
5	E	30	0	0	10	0
5	F	31	0	0	8	0
5	G	22	0	0	7	0
5	H	21	0	0	7	0
5	I	27	0	0	8	0
5	J	15	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28138	0	26750	507	1

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 9.

All (507) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:278:LYS:HA	5:B:6021:HOH:O	1.22	1.29
1:B:344:THR:HG21	5:B:6024:HOH:O	1.44	1.18
1:B:271:GLU:OE1	5:B:6016:HOH:O	1.63	1.14
1:D:123:GLU:HA	5:D:6013:HOH:O	1.54	1.05
1:J:117:PRO:HD2	5:J:6022:HOH:O	1.57	1.03
1:F:154:GLN:HE22	1:F:244:ASN:H	1.08	0.99
1:B:154:GLN:HE22	1:B:244:ASN:H	1.10	0.98
1:E:104:THR:HA	5:E:6025:HOH:O	1.60	0.98
1:A:154:GLN:HE22	1:A:244:ASN:H	1.08	0.97
1:I:154:GLN:HE22	1:I:244:ASN:H	1.09	0.96
1:E:154:GLN:HE22	1:E:244:ASN:H	1.07	0.96
1:H:154:GLN:HE22	1:H:244:ASN:H	1.14	0.95
1:J:154:GLN:HE22	1:J:244:ASN:H	1.14	0.93
1:C:154:GLN:HE22	1:C:244:ASN:H	1.08	0.93
3:A:5001:P3P:O13	3:A:5001:P3P:CEP	2.15	0.92
1:F:223:ARG:NH2	5:F:6030:HOH:O	2.02	0.90
1:D:154:GLN:HE22	1:D:244:ASN:H	1.11	0.90
1:G:154:GLN:HE22	1:G:244:ASN:H	1.10	0.89
1:E:297:GLU:OE2	3:E:5005:P3P:HEP3	1.75	0.87
1:E:106:LYS:HE2	5:E:6025:HOH:O	1.73	0.87
1:E:344:THR:HG21	5:E:6013:HOH:O	1.73	0.86
3:A:5001:P3P:O13	3:A:5001:P3P:HEP2	1.75	0.85
1:G:311:ARG:NH1	3:G:5006:P3P:O14	2.10	0.84
1:D:269:ALA:HA	5:D:6034:HOH:O	1.77	0.83
1:I:83:ARG:HG2	5:I:6030:HOH:O	1.77	0.83
1:E:205:SER:HA	5:E:6020:HOH:O	1.85	0.76
1:C:277:HIS:HE1	1:C:301:ILE:O	1.69	0.75
1:E:278:LYS:HE3	5:E:6030:HOH:O	1.86	0.75
1:G:277:HIS:HE1	1:G:301:ILE:O	1.69	0.75
1:F:277:HIS:HE1	1:F:301:ILE:O	1.70	0.75
1:D:311:ARG:HD3	3:D:5004:P3P:OEA	1.86	0.74
1:J:277:HIS:HE1	1:J:301:ILE:O	1.71	0.74
1:I:277:HIS:HE1	1:I:301:ILE:O	1.72	0.72
1:C:105:ASN:HD22	1:C:105:ASN:C	1.93	0.72
1:A:277:HIS:HE1	1:A:301:ILE:O	1.72	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:277:HIS:HE1	1:B:301:ILE:O	1.72	0.72
1:B:105:ASN:HD22	1:B:105:ASN:C	1.93	0.72
1:D:277:HIS:HE1	1:D:301:ILE:O	1.70	0.72
1:E:277:HIS:HE1	1:E:301:ILE:O	1.72	0.71
1:J:105:ASN:HD22	1:J:105:ASN:C	1.94	0.71
1:E:105:ASN:C	1:E:105:ASN:HD22	1.94	0.71
1:F:154:GLN:NE2	1:F:244:ASN:H	1.88	0.71
1:H:277:HIS:HE1	1:H:301:ILE:O	1.74	0.70
1:H:105:ASN:HD22	1:H:105:ASN:C	1.95	0.70
1:I:154:GLN:NE2	1:I:244:ASN:H	1.87	0.70
1:H:49:LYS:HE2	5:H:6025:HOH:O	1.92	0.70
1:A:105:ASN:HD22	1:A:105:ASN:C	1.95	0.70
1:F:20:ILE:O	5:F:6026:HOH:O	2.09	0.69
1:F:105:ASN:HD22	1:F:105:ASN:C	1.95	0.69
1:B:154:GLN:NE2	1:B:244:ASN:H	1.88	0.69
1:B:338:MET:HG3	1:B:343:VAL:HG21	1.74	0.69
1:D:123:GLU:CG	5:D:6013:HOH:O	2.40	0.69
1:A:347:ILE:O	1:A:351:THR:HB	1.93	0.68
1:E:154:GLN:NE2	1:E:244:ASN:H	1.87	0.68
1:F:347:ILE:O	1:F:351:THR:HB	1.94	0.68
1:I:105:ASN:HD22	1:I:105:ASN:C	1.96	0.67
1:B:347:ILE:O	1:B:351:THR:HB	1.95	0.67
1:H:49:LYS:CE	5:H:6025:HOH:O	2.41	0.67
1:A:122:GLU:HA	5:A:6017:HOH:O	1.95	0.67
1:D:296:HIS:HD2	5:D:6023:HOH:O	1.78	0.66
1:G:105:ASN:HD22	1:G:105:ASN:C	1.99	0.66
1:D:347:ILE:O	1:D:351:THR:HB	1.96	0.66
1:A:118:GLU:HB2	5:A:6008:HOH:O	1.95	0.66
1:H:232:VAL:HG23	5:H:6023:HOH:O	1.95	0.66
1:D:105:ASN:HD22	1:D:105:ASN:C	1.99	0.66
1:A:154:GLN:NE2	1:A:244:ASN:H	1.89	0.65
1:F:321:THR:CG2	5:F:6033:HOH:O	2.44	0.65
1:F:321:THR:HG23	5:F:6033:HOH:O	1.96	0.65
1:C:297:GLU:OE2	3:C:5003:P3P:HEP3	1.96	0.65
1:F:129:GLU:OE2	4:F:6007:ADP:O2A	2.14	0.65
1:F:129:GLU:HB3	5:F:6014:HOH:O	1.95	0.65
1:I:347:ILE:O	1:I:351:THR:HB	1.97	0.65
1:C:154:GLN:NE2	1:C:244:ASN:H	1.88	0.64
1:F:338:MET:HG3	1:F:343:VAL:HG21	1.79	0.64
1:G:347:ILE:O	1:G:351:THR:HB	1.98	0.64
1:D:332:ARG:HB2	5:D:6016:HOH:O	1.97	0.64
1:J:338:MET:HG3	1:J:343:VAL:HG21	1.79	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:321:THR:HB	1:D:327:GLY:HA3	1.78	0.64
1:C:347:ILE:O	1:C:351:THR:HB	1.98	0.64
1:D:338:MET:HG3	1:D:343:VAL:HG21	1.79	0.64
1:F:277:HIS:CD2	1:F:333:ARG:HH11	2.16	0.64
1:H:321:THR:HB	1:H:327:GLY:HA3	1.79	0.63
1:H:347:ILE:O	1:H:351:THR:HB	1.98	0.63
1:E:338:MET:HG3	1:E:343:VAL:HG21	1.80	0.63
1:G:154:GLN:NE2	1:G:244:ASN:H	1.90	0.63
1:E:169:ARG:HB3	5:E:6028:HOH:O	1.97	0.63
1:I:206:VAL:HG13	5:I:6017:HOH:O	1.98	0.63
3:F:5007:P3P:O13	3:F:5007:P3P:HEP1	1.98	0.63
1:D:154:GLN:NE2	1:D:244:ASN:H	1.91	0.63
1:C:338:MET:HG3	1:C:343:VAL:HG21	1.80	0.63
1:F:297:GLU:OE2	3:F:5007:P3P:HEP3	2.00	0.62
1:C:321:THR:HB	1:C:327:GLY:HA3	1.82	0.62
1:F:153:PRO:HA	5:F:6011:HOH:O	1.98	0.62
1:B:311:ARG:HD3	3:B:5002:P3P:OEA	2.00	0.62
1:G:321:THR:HB	1:G:327:GLY:HA3	1.82	0.62
1:D:311:ARG:NH1	3:D:5004:P3P:O14	2.32	0.61
1:E:347:ILE:O	1:E:351:THR:HB	2.00	0.61
1:J:347:ILE:O	1:J:351:THR:HB	1.99	0.61
1:G:111:ALA:HB3	5:G:6025:HOH:O	1.99	0.61
1:I:338:MET:HG3	1:I:343:VAL:HG21	1.82	0.61
1:A:338:MET:HG3	1:A:343:VAL:HG21	1.83	0.61
1:F:321:THR:HB	1:F:327:GLY:HA3	1.83	0.61
1:G:338:MET:HG3	1:G:343:VAL:HG21	1.83	0.61
1:H:223:ARG:NH2	5:H:6011:HOH:O	2.29	0.61
1:I:321:THR:HB	1:I:327:GLY:HA3	1.82	0.60
1:H:277:HIS:CD2	1:H:333:ARG:HH11	2.20	0.60
1:J:321:THR:HB	1:J:327:GLY:HA3	1.83	0.60
1:I:203:GLY:HA2	4:I:6008:ADP:O3'	2.02	0.60
1:H:338:MET:HG3	1:H:343:VAL:HG21	1.84	0.60
1:C:277:HIS:CD2	1:C:333:ARG:HH11	2.19	0.60
1:A:321:THR:HB	1:A:327:GLY:HA3	1.84	0.60
1:E:321:THR:HB	1:E:327:GLY:HA3	1.83	0.60
1:B:321:THR:HB	1:B:327:GLY:HA3	1.83	0.59
1:B:192:GLU:HB3	1:B:197:GLN:HE21	1.66	0.59
1:C:311:ARG:HD3	3:C:5003:P3P:OEA	2.02	0.59
1:E:351:THR:HG22	1:E:352:ILE:HG13	1.84	0.59
1:I:277:HIS:CD2	1:I:333:ARG:HH11	2.21	0.59
1:A:131:GLU:OE1	3:A:5001:P3P:HBP2	2.03	0.59
1:J:277:HIS:CD2	1:J:333:ARG:HH11	2.19	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:192:GLU:HB3	1:E:197:GLN:HE21	1.68	0.59
1:H:154:GLN:NE2	1:H:244:ASN:H	1.92	0.59
1:A:311:ARG:NH1	3:A:5001:P3P:O14	2.36	0.59
1:I:278:LYS:HB2	5:I:6018:HOH:O	2.02	0.58
1:D:192:GLU:HB3	1:D:197:GLN:HE21	1.69	0.58
1:B:277:HIS:CD2	1:B:333:ARG:HH11	2.20	0.58
1:G:277:HIS:CD2	1:G:333:ARG:HH11	2.20	0.58
1:D:156:PRO:HB3	5:D:6018:HOH:O	2.03	0.58
1:I:192:GLU:HB3	1:I:197:GLN:HE21	1.68	0.58
1:G:192:GLU:HB3	1:G:197:GLN:HE21	1.69	0.58
1:I:296:HIS:HD2	5:I:6034:HOH:O	1.85	0.58
1:D:351:THR:HG22	1:D:352:ILE:HG13	1.86	0.58
1:I:351:THR:HG22	1:I:352:ILE:HG13	1.86	0.58
1:E:137:LYS:O	1:E:138:ASP:HB2	2.04	0.57
1:E:277:HIS:CD2	1:E:333:ARG:HH11	2.21	0.57
1:C:192:GLU:HB3	1:C:197:GLN:HE21	1.70	0.57
1:C:351:THR:HG22	1:C:352:ILE:HG13	1.86	0.57
1:A:277:HIS:CD2	1:A:333:ARG:HH11	2.23	0.57
5:D:6030:HOH:O	1:E:190:ASN:HA	2.04	0.56
1:G:41:PRO:HB3	5:G:6027:HOH:O	2.06	0.56
1:E:318:GLY:HA3	5:E:6007:HOH:O	2.04	0.56
1:D:277:HIS:CD2	1:D:333:ARG:HH11	2.24	0.56
1:G:351:THR:HG22	1:G:352:ILE:HG13	1.88	0.56
1:A:192:GLU:HB3	1:A:197:GLN:HE21	1.71	0.56
1:A:351:THR:HG22	1:A:352:ILE:HG13	1.88	0.55
1:J:192:GLU:HB3	1:J:197:GLN:HE21	1.71	0.55
3:I:5008:P3P:O14	4:I:6008:ADP:O3B	2.24	0.55
1:H:311:ARG:HD3	3:H:5010:P3P:OEA	2.05	0.55
1:J:154:GLN:NE2	1:J:244:ASN:H	1.94	0.55
1:F:351:THR:HG22	1:F:352:ILE:HG13	1.89	0.55
1:A:121:ALA:O	5:A:6017:HOH:O	2.17	0.55
1:G:296:HIS:HB2	5:G:6012:HOH:O	2.07	0.55
1:B:297:GLU:OE2	3:B:5002:P3P:HEP3	2.07	0.55
1:A:121:ALA:C	5:A:6017:HOH:O	2.44	0.55
1:H:351:THR:HG22	1:H:352:ILE:HG13	1.89	0.54
1:D:316:ARG:NH1	1:D:330:GLU:OE1	2.38	0.54
1:A:316:ARG:NH1	1:A:330:GLU:OE1	2.38	0.54
1:B:351:THR:HG22	1:B:352:ILE:HG13	1.88	0.54
1:D:123:GLU:HG2	5:D:6013:HOH:O	2.05	0.54
4:G:6006:ADP:O2A	4:G:6006:ADP:O3B	2.25	0.54
1:D:252:TYR:HE1	1:D:351:THR:HG21	1.73	0.54
1:I:131:GLU:OE1	3:I:5008:P3P:HGP1	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:264:GLU:HB3	5:B:6027:HOH:O	2.06	0.54
1:G:73:TYR:CD2	1:G:95:TYR:CE1	2.96	0.54
1:F:129:GLU:CD	4:F:6007:ADP:O2A	2.47	0.53
1:J:137:LYS:O	1:J:138:ASP:HB2	2.08	0.53
1:H:192:GLU:HB3	1:H:197:GLN:HE21	1.72	0.53
1:F:137:LYS:O	1:F:138:ASP:HB2	2.07	0.53
1:D:203:GLY:HA2	4:D:6005:ADP:O3'	2.09	0.53
1:C:333:ARG:N	1:C:334:PRO:CD	2.71	0.53
1:I:252:TYR:HE1	1:I:351:THR:HG21	1.74	0.53
1:F:192:GLU:HB3	1:F:197:GLN:HE21	1.73	0.53
1:I:218:ARG:HB3	5:I:6009:HOH:O	2.08	0.53
1:J:351:THR:HG22	1:J:352:ILE:HG13	1.91	0.52
1:D:56:ASP:OD2	3:E:5005:P3P:HEP1	2.09	0.52
1:E:272:LYS:HE3	5:E:6026:HOH:O	2.10	0.52
1:E:73:TYR:CD2	1:E:95:TYR:CE1	2.98	0.52
1:J:340:PRO:O	1:J:344:THR:HB	2.09	0.52
1:D:252:TYR:CE1	1:D:351:THR:HG21	2.44	0.52
1:F:73:TYR:CD2	1:F:95:TYR:CE1	2.98	0.52
1:H:172:VAL:HG21	1:H:198:TRP:CD2	2.45	0.52
1:B:172:VAL:HG21	1:B:198:TRP:CD2	2.45	0.52
1:A:73:TYR:CD2	1:A:95:TYR:CE1	2.98	0.52
1:F:340:PRO:O	1:F:344:THR:HB	2.10	0.52
1:B:131:GLU:OE1	3:B:5002:P3P:HBP2	2.10	0.51
1:D:192:GLU:OE1	3:D:5004:P3P:HEP2	2.10	0.51
1:A:252:TYR:CE1	1:A:351:THR:HG21	2.45	0.51
1:A:252:TYR:HE1	1:A:351:THR:HG21	1.75	0.51
1:J:252:TYR:HE1	1:J:351:THR:HG21	1.75	0.51
1:I:137:LYS:O	1:I:138:ASP:HB2	2.10	0.51
3:F:5007:P3P:O13	3:F:5007:P3P:CEP	2.58	0.51
1:I:19:ILE:HD11	1:I:86:ASN:HB2	1.93	0.51
1:J:275:LEU:HD21	5:J:6014:HOH:O	2.10	0.51
1:D:272:LYS:HE3	5:D:6034:HOH:O	2.10	0.51
1:A:352:ILE:HA	5:A:6007:HOH:O	2.10	0.51
1:E:292:LEU:HD23	1:E:298:THR:HB	1.93	0.51
1:I:316:ARG:NH1	1:I:330:GLU:OE1	2.42	0.51
1:D:137:LYS:O	1:D:138:ASP:HB2	2.11	0.51
1:I:252:TYR:CE1	1:I:351:THR:HG21	2.46	0.51
1:C:73:TYR:CD2	1:C:95:TYR:CE1	2.98	0.51
1:G:203:GLY:HA2	4:G:6006:ADP:O3'	2.10	0.51
1:D:73:TYR:CD2	1:D:95:TYR:CE1	2.99	0.51
1:F:252:TYR:HE1	1:F:351:THR:HG21	1.76	0.51
1:F:248:ALA:HB1	1:F:338:MET:HE3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:137:LYS:O	1:C:138:ASP:HB2	2.10	0.51
1:F:316:ARG:NH1	1:F:330:GLU:OE1	2.39	0.51
1:D:172:VAL:HG21	1:D:198:TRP:CD2	2.46	0.51
1:E:38:ARG:HB3	1:E:53:TRP:CH2	2.46	0.50
1:H:137:LYS:O	1:H:138:ASP:HB2	2.09	0.50
1:F:172:VAL:HG21	1:F:198:TRP:CD2	2.47	0.50
1:G:137:LYS:O	1:G:138:ASP:HB2	2.11	0.50
1:I:73:TYR:CD2	1:I:95:TYR:CE1	2.99	0.50
1:C:105:ASN:HD21	1:C:108:TYR:H	1.60	0.50
1:E:142:PRO:HB2	1:E:145:TRP:CD1	2.46	0.50
1:D:46:ASP:HB2	5:D:6009:HOH:O	2.11	0.50
1:C:248:ALA:HB1	1:C:338:MET:HE3	1.92	0.50
1:J:252:TYR:CE1	1:J:351:THR:HG21	2.47	0.50
1:D:19:ILE:HD11	1:D:86:ASN:HB2	1.93	0.50
3:A:5001:P3P:HEP1	3:A:5001:P3P:O13	2.07	0.50
1:I:248:ALA:HB1	1:I:338:MET:HE3	1.94	0.50
1:D:333:ARG:N	1:D:334:PRO:CD	2.75	0.50
1:A:292:LEU:HD23	1:A:298:THR:HB	1.94	0.50
1:A:137:LYS:O	1:A:138:ASP:HB2	2.12	0.50
1:G:292:LEU:HD23	1:G:298:THR:HB	1.94	0.49
1:B:292:LEU:HD23	1:B:298:THR:HB	1.94	0.49
1:H:73:TYR:CD2	1:H:95:TYR:CE1	3.00	0.49
1:E:172:VAL:HG21	1:E:198:TRP:CD2	2.46	0.49
1:A:172:VAL:HG21	1:A:198:TRP:CD2	2.46	0.49
1:H:192:GLU:OE1	3:H:5010:P3P:HEP2	2.12	0.49
1:I:305:SER:H	1:I:314:SER:HB2	1.77	0.49
1:J:272:LYS:HE3	5:J:6023:HOH:O	2.12	0.49
1:C:105:ASN:C	1:C:105:ASN:ND2	2.64	0.49
1:C:105:ASN:ND2	1:C:108:TYR:H	2.09	0.49
1:C:223:ARG:NH1	5:C:6007:HOH:O	2.44	0.49
1:G:172:VAL:HG21	1:G:198:TRP:CD2	2.48	0.49
1:D:38:ARG:HB3	1:D:53:TRP:CH2	2.47	0.49
1:E:252:TYR:HE1	1:E:351:THR:HG21	1.77	0.49
1:G:129:GLU:HB3	5:G:6018:HOH:O	2.13	0.49
1:F:252:TYR:CE1	1:F:351:THR:HG21	2.48	0.49
1:C:192:GLU:OE1	3:C:5003:P3P:HEP2	2.11	0.49
1:A:340:PRO:O	1:A:344:THR:HB	2.13	0.49
1:F:292:LEU:HD23	1:F:298:THR:HB	1.94	0.49
1:B:105:ASN:ND2	1:B:105:ASN:C	2.65	0.49
1:B:252:TYR:CE1	1:B:351:THR:HG21	2.48	0.49
1:F:236:PRO:HB3	1:F:335:ALA:HB1	1.94	0.49
1:B:301:ILE:H	1:B:301:ILE:HG13	1.39	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:248:ALA:HB1	1:H:338:MET:HE3	1.94	0.49
1:F:129:GLU:CB	5:F:6014:HOH:O	2.59	0.48
1:G:273:LEU:O	5:G:6009:HOH:O	2.19	0.48
1:A:142:PRO:HB2	1:A:145:TRP:CD1	2.48	0.48
1:A:333:ARG:N	1:A:334:PRO:CD	2.76	0.48
1:B:252:TYR:HE1	1:B:351:THR:HG21	1.77	0.48
1:F:301:ILE:HG13	1:F:301:ILE:H	1.47	0.48
1:J:305:SER:H	1:J:314:SER:HB2	1.79	0.48
1:C:292:LEU:HD23	1:C:298:THR:HB	1.95	0.48
1:C:333:ARG:N	1:C:334:PRO:HD3	2.29	0.48
1:D:105:ASN:ND2	1:D:108:TYR:H	2.10	0.48
1:I:296:HIS:CD2	5:I:6034:HOH:O	2.63	0.48
1:I:142:PRO:HB2	1:I:145:TRP:CD1	2.48	0.48
1:G:248:ALA:HB1	1:G:338:MET:HE3	1.96	0.48
1:D:248:ALA:HB1	1:D:338:MET:HE3	1.96	0.48
1:A:248:ALA:HB1	1:A:338:MET:HE3	1.94	0.48
1:I:172:VAL:HG21	1:I:198:TRP:CD2	2.48	0.48
1:H:316:ARG:NH1	1:H:330:GLU:OE1	2.44	0.48
1:E:105:ASN:ND2	1:E:105:ASN:C	2.66	0.48
1:E:252:TYR:CE1	1:E:351:THR:HG21	2.48	0.48
1:J:203:GLY:HA2	4:J:6009:ADP:O3'	2.13	0.48
1:F:333:ARG:N	1:F:334:PRO:CD	2.76	0.48
1:G:340:PRO:O	1:G:344:THR:HB	2.13	0.48
1:C:172:VAL:HG21	1:C:198:TRP:CD2	2.49	0.48
1:J:73:TYR:CD2	1:J:95:TYR:CE1	3.02	0.48
1:H:49:LYS:HE3	5:H:6025:HOH:O	2.10	0.47
1:C:236:PRO:HB3	1:C:335:ALA:HB1	1.95	0.47
1:I:340:PRO:O	1:I:344:THR:HB	2.14	0.47
1:B:19:ILE:HD11	1:B:86:ASN:HB2	1.96	0.47
1:D:105:ASN:HD21	1:D:108:TYR:H	1.60	0.47
1:C:135:LEU:HD23	1:C:142:PRO:HA	1.96	0.47
1:E:129:GLU:HB2	5:E:6022:HOH:O	2.14	0.47
1:I:333:ARG:N	1:I:334:PRO:CD	2.77	0.47
1:C:252:TYR:HE1	1:C:351:THR:HG21	1.79	0.47
1:H:252:TYR:HE1	1:H:351:THR:HG21	1.79	0.47
1:I:236:PRO:HB3	1:I:335:ALA:HB1	1.94	0.47
1:J:142:PRO:HB2	1:J:145:TRP:CD1	2.50	0.47
1:I:301:ILE:H	1:I:301:ILE:HG13	1.40	0.47
1:E:333:ARG:N	1:E:334:PRO:CD	2.78	0.47
1:I:292:LEU:HD23	1:I:298:THR:HB	1.96	0.47
1:J:105:ASN:ND2	1:J:105:ASN:C	2.65	0.47
1:F:105:ASN:ND2	1:F:105:ASN:C	2.66	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:252:TYR:HE1	1:G:351:THR:HG21	1.78	0.47
1:G:252:TYR:CE1	1:G:351:THR:HG21	2.49	0.47
1:H:142:PRO:HB2	1:H:145:TRP:CD1	2.49	0.47
1:C:305:SER:H	1:C:314:SER:HB2	1.79	0.47
1:B:105:ASN:ND2	1:B:108:TYR:H	2.12	0.47
1:D:135:LEU:HD23	1:D:142:PRO:HA	1.97	0.47
1:J:172:VAL:HG21	1:J:198:TRP:CD2	2.49	0.47
1:B:271:GLU:CD	5:B:6016:HOH:O	2.36	0.47
1:F:88:ILE:N	5:F:6026:HOH:O	2.48	0.47
1:C:252:TYR:CE1	1:C:351:THR:HG21	2.50	0.47
1:E:248:ALA:HB1	1:E:338:MET:HE3	1.96	0.47
1:G:333:ARG:N	1:G:334:PRO:CD	2.78	0.46
1:B:38:ARG:HB3	1:B:53:TRP:CH2	2.50	0.46
1:H:340:PRO:O	1:H:344:THR:HB	2.15	0.46
1:F:142:PRO:HB2	1:F:145:TRP:CD1	2.51	0.46
1:C:340:PRO:O	1:C:344:THR:HB	2.15	0.46
1:H:38:ARG:HB3	1:H:53:TRP:CH2	2.49	0.46
1:D:292:LEU:HD23	1:D:298:THR:HB	1.96	0.46
1:J:301:ILE:H	1:J:301:ILE:HG13	1.43	0.46
1:G:316:ARG:NH1	1:G:330:GLU:OE1	2.43	0.46
1:A:105:ASN:ND2	1:A:105:ASN:C	2.67	0.46
1:H:252:TYR:CE1	1:H:351:THR:HG21	2.50	0.46
1:A:36:LYS:NZ	5:A:6003:HOH:O	2.48	0.46
3:E:5005:P3P:OEA	3:E:5005:P3P:O14	2.34	0.46
1:B:105:ASN:HD21	1:B:108:TYR:H	1.62	0.46
1:H:333:ARG:N	1:H:334:PRO:CD	2.78	0.46
1:G:105:ASN:ND2	1:G:108:TYR:H	2.12	0.46
1:A:19:ILE:HD11	1:A:86:ASN:HB2	1.98	0.46
1:I:96:THR:HB	1:I:97:PRO:CD	2.45	0.46
1:D:236:PRO:HB3	1:D:335:ALA:HB1	1.97	0.46
1:H:305:SER:H	1:H:314:SER:HB2	1.81	0.46
1:J:38:ARG:HB3	1:J:53:TRP:CH2	2.51	0.46
1:I:291:ARG:NH1	3:I:5008:P3P:OP	2.49	0.46
1:C:316:ARG:NH1	1:C:330:GLU:OE1	2.45	0.46
1:H:4:LEU:HD12	1:H:4:LEU:HA	1.84	0.46
1:G:277:HIS:HD2	1:G:333:ARG:HH11	1.62	0.46
1:B:316:ARG:NH1	1:B:330:GLU:OE1	2.42	0.46
1:A:38:ARG:HB3	1:A:53:TRP:CH2	2.51	0.46
1:B:116:SER:HA	1:B:117:PRO:HD3	1.78	0.46
1:I:105:ASN:ND2	1:I:108:TYR:H	2.13	0.46
1:G:135:LEU:HD23	1:G:142:PRO:HA	1.97	0.46
1:A:236:PRO:HB3	1:A:335:ALA:HB1	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:236:PRO:HB3	1:G:335:ALA:HB1	1.98	0.46
1:B:73:TYR:CD2	1:B:95:TYR:CE1	3.04	0.46
1:B:236:PRO:HB3	1:B:335:ALA:HB1	1.98	0.46
1:G:38:ARG:HB3	1:G:53:TRP:CH2	2.50	0.46
1:C:38:ARG:HB3	1:C:53:TRP:CH2	2.52	0.46
1:H:135:LEU:HD23	1:H:142:PRO:HA	1.99	0.45
1:B:135:LEU:HD23	1:B:142:PRO:HA	1.98	0.45
1:E:236:PRO:HB3	1:E:335:ALA:HB1	1.97	0.45
1:F:277:HIS:HD2	1:F:333:ARG:HH11	1.62	0.45
1:B:333:ARG:N	1:B:334:PRO:CD	2.80	0.45
1:I:249:HIS:HE1	3:I:5008:P3P:OEB	2.00	0.45
1:H:236:PRO:HB3	1:H:335:ALA:HB1	1.99	0.45
1:I:105:ASN:ND2	1:I:105:ASN:C	2.67	0.45
1:H:280:HIS:CG	5:H:6031:HOH:O	2.69	0.45
1:D:96:THR:HB	1:D:97:PRO:CD	2.47	0.45
1:F:19:ILE:HD11	1:F:86:ASN:HB2	1.99	0.45
1:A:333:ARG:N	1:A:334:PRO:HD3	2.32	0.45
1:E:305:SER:H	1:E:314:SER:HB2	1.81	0.45
1:E:96:THR:HB	1:E:97:PRO:CD	2.47	0.45
1:D:4:LEU:HA	1:D:4:LEU:HD12	1.81	0.45
1:A:135:LEU:HD23	1:A:142:PRO:HA	1.98	0.45
1:I:116:SER:HA	1:I:117:PRO:HD3	1.77	0.45
1:B:142:PRO:HB2	1:B:145:TRP:CD1	2.52	0.44
1:B:235:ASP:OD2	1:B:290:ARG:NH2	2.50	0.44
1:I:38:ARG:HB3	1:I:53:TRP:CH2	2.52	0.44
1:F:305:SER:H	1:F:314:SER:HB2	1.82	0.44
1:B:137:LYS:O	1:B:138:ASP:HB2	2.17	0.44
1:J:248:ALA:HB1	1:J:338:MET:HE3	1.99	0.44
1:D:340:PRO:O	1:D:344:THR:HB	2.17	0.44
1:D:280:HIS:NE2	1:D:346:MET:HG2	2.32	0.44
1:J:292:LEU:HD23	1:J:298:THR:HB	1.99	0.44
1:G:105:ASN:HD21	1:G:108:TYR:H	1.64	0.44
1:G:19:ILE:HD11	1:G:86:ASN:HB2	1.99	0.44
1:A:305:SER:H	1:A:314:SER:HB2	1.82	0.44
1:D:333:ARG:N	1:D:334:PRO:HD3	2.32	0.44
1:A:122:GLU:CA	5:A:6017:HOH:O	2.62	0.44
1:G:142:PRO:HB2	1:G:145:TRP:CD1	2.51	0.44
1:C:4:LEU:HD12	1:C:4:LEU:HA	1.81	0.44
1:A:96:THR:HB	1:A:97:PRO:CD	2.47	0.44
1:I:204:PRO:HD2	5:I:6029:HOH:O	2.17	0.44
1:J:105:ASN:ND2	1:J:108:TYR:H	2.15	0.44
1:H:105:ASN:ND2	1:H:108:TYR:H	2.16	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:116:SER:HA	1:D:117:PRO:HD3	1.77	0.44
1:D:235:ASP:OD2	1:D:290:ARG:NH2	2.50	0.44
1:F:105:ASN:ND2	1:F:108:TYR:H	2.16	0.44
1:C:24:ILE:O	1:C:92:CYS:HB2	2.18	0.44
1:I:355:LYS:HB2	5:I:6016:HOH:O	2.18	0.44
1:H:116:SER:HA	1:H:117:PRO:HD3	1.71	0.44
1:H:292:LEU:HD23	1:H:298:THR:HB	1.98	0.44
1:B:305:SER:H	1:B:314:SER:HB2	1.82	0.44
1:B:248:ALA:HB1	1:B:338:MET:HE3	1.99	0.44
1:I:135:LEU:HD23	1:I:142:PRO:HA	1.99	0.44
1:E:19:ILE:HD11	1:E:86:ASN:HB2	2.00	0.44
1:F:116:SER:HA	1:F:117:PRO:HD3	1.75	0.44
1:A:235:ASP:OD2	1:A:290:ARG:NH2	2.51	0.44
1:D:301:ILE:H	1:D:301:ILE:HG13	1.43	0.44
1:C:19:ILE:HD11	1:C:86:ASN:HB2	2.00	0.44
1:E:116:SER:HA	1:E:117:PRO:HD3	1.76	0.43
1:I:333:ARG:N	1:I:334:PRO:HD3	2.33	0.43
1:E:135:LEU:HD23	1:E:142:PRO:HA	2.00	0.43
1:F:135:LEU:HD23	1:F:142:PRO:HA	2.00	0.43
1:B:340:PRO:O	1:B:344:THR:HB	2.18	0.43
1:I:105:ASN:HD21	1:I:108:TYR:H	1.65	0.43
1:G:305:SER:H	1:G:314:SER:HB2	1.82	0.43
1:D:305:SER:H	1:D:314:SER:HB2	1.83	0.43
1:J:316:ARG:NH1	1:J:330:GLU:OE1	2.45	0.43
1:G:297:GLU:OE2	3:G:5006:P3P:HEP3	2.18	0.43
1:H:105:ASN:HD21	1:H:108:TYR:H	1.65	0.43
1:J:277:HIS:HD2	1:J:333:ARG:HH11	1.62	0.43
1:J:105:ASN:HD21	1:J:108:TYR:H	1.65	0.43
1:I:235:ASP:OD2	1:I:290:ARG:NH2	2.52	0.43
1:J:12:LEU:HD23	1:J:12:LEU:HA	1.88	0.43
1:C:116:SER:HA	1:C:117:PRO:HD3	1.77	0.43
1:B:127:GLY:HA3	4:B:6002:ADP:H1'	1.99	0.43
1:J:238:PRO:O	1:J:239:ILE:HD13	2.19	0.43
1:J:157:TYR:CD1	1:J:195:PRO:HD3	2.54	0.43
1:J:19:ILE:HD11	1:J:86:ASN:HB2	1.99	0.43
1:G:115:SER:CB	5:G:6015:HOH:O	2.67	0.43
1:G:116:SER:HA	1:G:117:PRO:HD3	1.77	0.43
1:D:142:PRO:HB2	1:D:145:TRP:CD1	2.53	0.43
1:E:301:ILE:H	1:E:301:ILE:HG13	1.44	0.43
1:H:105:ASN:C	1:H:105:ASN:ND2	2.66	0.43
1:B:96:THR:HB	1:B:97:PRO:CD	2.48	0.43
1:I:157:TYR:CD1	1:I:195:PRO:HD3	2.54	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:236:PRO:HB3	1:J:335:ALA:HB1	2.00	0.43
1:C:277:HIS:HD2	1:C:333:ARG:HH11	1.63	0.42
1:A:105:ASN:ND2	1:A:108:TYR:H	2.16	0.42
1:I:277:HIS:HD2	1:I:333:ARG:HH11	1.67	0.42
1:H:277:HIS:HD2	1:H:333:ARG:HH11	1.64	0.42
1:D:105:ASN:C	1:D:105:ASN:ND2	2.70	0.42
1:F:311:ARG:NH1	3:F:5007:P3P:O13	2.52	0.42
1:A:4:LEU:HA	1:A:4:LEU:HD12	1.85	0.42
1:J:116:SER:HA	1:J:117:PRO:HD3	1.77	0.42
1:J:333:ARG:N	1:J:334:PRO:CD	2.81	0.42
1:E:277:HIS:HD2	1:E:333:ARG:HH11	1.66	0.42
1:G:284:TYR:CD2	1:G:343:VAL:HG22	2.55	0.42
1:E:105:ASN:ND2	1:E:108:TYR:H	2.16	0.42
1:F:235:ASP:OD2	1:F:290:ARG:NH2	2.53	0.42
1:J:24:ILE:O	1:J:92:CYS:HB2	2.19	0.42
1:A:116:SER:HA	1:A:117:PRO:HD3	1.75	0.42
1:A:3:CYS:HB2	1:A:4:LEU:H	1.75	0.42
1:B:230:VAL:CG1	1:B:231:VAL:N	2.82	0.42
1:D:10:LEU:HD23	1:D:10:LEU:HA	1.90	0.42
1:F:333:ARG:N	1:F:334:PRO:HD3	2.35	0.42
1:C:102:ILE:HB	1:C:103:PRO:CD	2.50	0.42
1:H:19:ILE:HD11	1:H:86:ASN:HB2	2.01	0.42
1:C:142:PRO:HB2	1:C:145:TRP:CD1	2.55	0.42
1:H:233:THR:HB	1:H:235:ASP:H	1.85	0.42
1:H:24:ILE:O	1:H:92:CYS:HB2	2.20	0.42
1:E:333:ARG:N	1:E:334:PRO:HD3	2.35	0.42
1:F:280:HIS:NE2	1:F:346:MET:HG2	2.35	0.42
1:C:281:ILE:HA	1:C:281:ILE:HD13	1.88	0.42
1:F:4:LEU:HA	1:F:4:LEU:HD12	1.83	0.42
1:G:96:THR:HB	1:G:97:PRO:CD	2.49	0.42
1:D:58:SER:HA	1:D:63:ALA:O	2.19	0.42
1:B:281:ILE:HA	1:B:281:ILE:HD13	1.89	0.42
1:H:56:ASP:OD1	1:H:56:ASP:C	2.58	0.42
1:H:301:ILE:H	1:H:301:ILE:HG13	1.42	0.41
1:H:3:CYS:HB2	1:H:4:LEU:H	1.78	0.41
1:I:355:LYS:HB2	1:I:355:LYS:HE2	1.91	0.41
1:B:203:GLY:HA2	4:B:6002:ADP:O3'	2.20	0.41
1:F:38:ARG:HB3	1:F:53:TRP:CH2	2.55	0.41
1:J:56:ASP:OD1	1:J:56:ASP:C	2.56	0.41
1:G:10:LEU:HD23	1:G:10:LEU:HA	1.91	0.41
1:F:96:THR:HB	1:F:97:PRO:CD	2.49	0.41
1:D:272:LYS:HG3	5:D:6034:HOH:O	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:180:LEU:HA	1:I:180:LEU:HD23	1.90	0.41
1:G:129:GLU:OE2	4:G:6006:ADP:O2A	2.39	0.41
1:I:105:ASN:ND2	1:I:107:ARG:H	2.18	0.41
1:I:284:TYR:CD2	1:I:343:VAL:HG22	2.56	0.41
1:J:96:THR:HB	1:J:97:PRO:CD	2.51	0.41
1:G:4:LEU:HD12	1:G:4:LEU:HA	1.82	0.41
1:G:115:SER:HB2	5:G:6015:HOH:O	2.19	0.41
1:B:333:ARG:N	1:B:334:PRO:HD3	2.36	0.41
1:H:235:ASP:OD2	1:H:290:ARG:NH2	2.53	0.41
1:F:102:ILE:HB	1:F:103:PRO:CD	2.51	0.41
1:F:84:ARG:HH11	1:F:84:ARG:HD2	1.74	0.41
1:J:235:ASP:OD2	1:J:290:ARG:NH2	2.54	0.41
1:E:105:ASN:HD21	1:E:108:TYR:H	1.68	0.41
1:A:105:ASN:HD21	1:A:108:TYR:H	1.68	0.41
1:F:105:ASN:HD21	1:F:108:TYR:H	1.68	0.41
1:C:131:GLU:OE1	3:C:5003:P3P:HBP2	2.21	0.41
1:A:284:TYR:CD2	1:A:343:VAL:HG22	2.55	0.41
1:I:233:THR:HB	1:I:235:ASP:H	1.86	0.41
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.91	0.41
1:I:3:CYS:HB2	1:I:4:LEU:H	1.80	0.41
1:G:288:ASN:HA	1:G:288:ASN:HD22	1.68	0.41
1:I:12:LEU:HD23	1:I:12:LEU:HA	1.92	0.41
1:C:235:ASP:OD2	1:C:290:ARG:NH2	2.53	0.41
1:E:3:CYS:HB2	1:E:4:LEU:H	1.80	0.41
1:E:316:ARG:NH1	1:E:330:GLU:OE1	2.44	0.41
1:G:284:TYR:CE2	1:G:343:VAL:HG22	2.56	0.41
1:C:280:HIS:NE2	1:C:346:MET:HG2	2.36	0.41
1:C:277:HIS:CE1	1:C:301:ILE:O	2.60	0.40
1:C:105:ASN:ND2	1:C:107:ARG:H	2.19	0.40
1:A:301:ILE:HG13	1:A:301:ILE:H	1.41	0.40
1:B:129:GLU:O	1:B:248:ALA:HA	2.21	0.40
1:G:105:ASN:C	1:G:105:ASN:ND2	2.70	0.40
1:E:238:PRO:O	1:E:239:ILE:HD13	2.21	0.40
1:J:284:TYR:CD2	1:J:343:VAL:HG22	2.56	0.40
1:G:180:LEU:HD23	1:G:180:LEU:HA	1.89	0.40
1:G:233:THR:HB	1:G:235:ASP:H	1.86	0.40
1:E:332:ARG:NH2	3:E:5005:P3P:O14	2.54	0.40
1:E:129:GLU:O	5:E:6022:HOH:O	2.22	0.40
1:D:230:VAL:CG1	1:D:231:VAL:N	2.84	0.40
1:B:80:ASP:C	1:B:80:ASP:OD1	2.59	0.40
1:G:333:ARG:N	1:G:334:PRO:HD3	2.37	0.40
1:D:314:SER:HB3	1:D:333:ARG:HD3	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:105:ASN:HD22	1:G:107:ARG:H	1.69	0.40
1:C:96:THR:HB	1:C:97:PRO:CD	2.51	0.40
1:H:103:PRO:HA	5:H:6027:HOH:O	2.20	0.40
1:B:39:THR:O	1:B:40:LEU:HD23	2.20	0.40
1:G:281:ILE:HA	1:G:281:ILE:HD13	1.83	0.40
1:F:80:ASP:C	1:F:80:ASP:OD1	2.60	0.40
1:I:102:ILE:HB	1:I:103:PRO:CD	2.52	0.40
1:B:141:TRP:HA	1:B:142:PRO:HD3	1.95	0.40
1:B:3:CYS:HB2	1:B:4:LEU:H	1.79	0.40
1:J:39:THR:O	1:J:40:LEU:HD23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:302:ASN:O	1:H:355:LYS:CB[2_655]	2.16	0.04

## 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	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	B	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	C	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	D	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	E	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	F	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	G	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	H	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	I	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	J	351/356 (99%)	336 (96%)	14 (4%)	1 (0%)	50	91
All	All	3510/3560 (99%)	3334 (95%)	175 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	203	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	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	B	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	C	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	D	288/290 (99%)	268 (93%)	20 (7%)	22	70
1	E	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	F	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	G	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	H	288/290 (99%)	266 (92%)	22 (8%)	19	67
1	I	288/290 (99%)	267 (93%)	21 (7%)	20	68
1	J	288/290 (99%)	267 (93%)	21 (7%)	20	68
All	All	2880/2900 (99%)	2670 (93%)	210 (7%)	20	68

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	CYS
1	A	19	ILE
1	A	45	THR
1	A	105	ASN
1	A	116	SER
1	A	128	ILE
1	A	143	LEU
1	A	164	GLU
1	A	176	TYR
1	A	201	GLN
1	A	206	VAL
1	A	232	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	233	THR
1	A	258	ARG
1	A	288	ASN
1	A	289	GLU
1	A	301	ILE
1	A	321	THR
1	A	338	MET
1	A	344	THR
1	A	351	THR
1	B	3	CYS
1	B	19	ILE
1	B	45	THR
1	B	105	ASN
1	B	116	SER
1	B	128	ILE
1	B	143	LEU
1	B	164	GLU
1	B	176	TYR
1	B	201	GLN
1	B	206	VAL
1	B	232	VAL
1	B	233	THR
1	B	258	ARG
1	B	288	ASN
1	B	289	GLU
1	B	301	ILE
1	B	321	THR
1	B	338	MET
1	B	344	THR
1	B	351	THR
1	C	3	CYS
1	C	19	ILE
1	C	45	THR
1	C	105	ASN
1	C	116	SER
1	C	128	ILE
1	C	143	LEU
1	C	164	GLU
1	C	176	TYR
1	C	201	GLN
1	C	206	VAL
1	C	232	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	233	THR
1	C	258	ARG
1	C	288	ASN
1	C	289	GLU
1	C	301	ILE
1	C	321	THR
1	C	338	MET
1	C	344	THR
1	C	351	THR
1	D	3	CYS
1	D	19	ILE
1	D	45	THR
1	D	105	ASN
1	D	116	SER
1	D	128	ILE
1	D	143	LEU
1	D	164	GLU
1	D	176	TYR
1	D	201	GLN
1	D	206	VAL
1	D	232	VAL
1	D	258	ARG
1	D	288	ASN
1	D	289	GLU
1	D	301	ILE
1	D	321	THR
1	D	338	MET
1	D	344	THR
1	D	351	THR
1	E	3	CYS
1	E	19	ILE
1	E	45	THR
1	E	105	ASN
1	E	116	SER
1	E	128	ILE
1	E	143	LEU
1	E	164	GLU
1	E	176	TYR
1	E	201	GLN
1	E	206	VAL
1	E	232	VAL
1	E	233	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	258	ARG
1	E	288	ASN
1	E	289	GLU
1	E	301	ILE
1	E	321	THR
1	E	338	MET
1	E	344	THR
1	E	351	THR
1	F	3	CYS
1	F	19	ILE
1	F	45	THR
1	F	105	ASN
1	F	116	SER
1	F	128	ILE
1	F	143	LEU
1	F	164	GLU
1	F	176	TYR
1	F	201	GLN
1	F	206	VAL
1	F	232	VAL
1	F	233	THR
1	F	258	ARG
1	F	288	ASN
1	F	289	GLU
1	F	301	ILE
1	F	321	THR
1	F	338	MET
1	F	344	THR
1	F	351	THR
1	G	3	CYS
1	G	19	ILE
1	G	45	THR
1	G	105	ASN
1	G	116	SER
1	G	128	ILE
1	G	143	LEU
1	G	164	GLU
1	G	176	TYR
1	G	201	GLN
1	G	206	VAL
1	G	232	VAL
1	G	233	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	258	ARG
1	G	288	ASN
1	G	289	GLU
1	G	301	ILE
1	G	321	THR
1	G	338	MET
1	G	344	THR
1	G	351	THR
1	H	3	CYS
1	H	19	ILE
1	H	45	THR
1	H	105	ASN
1	H	116	SER
1	H	128	ILE
1	H	143	LEU
1	H	164	GLU
1	H	176	TYR
1	H	201	GLN
1	H	204	PRO
1	H	206	VAL
1	H	232	VAL
1	H	233	THR
1	H	258	ARG
1	H	288	ASN
1	H	289	GLU
1	H	301	ILE
1	H	321	THR
1	H	338	MET
1	H	344	THR
1	H	351	THR
1	I	3	CYS
1	I	19	ILE
1	I	45	THR
1	I	105	ASN
1	I	116	SER
1	I	128	ILE
1	I	143	LEU
1	I	164	GLU
1	I	176	TYR
1	I	201	GLN
1	I	206	VAL
1	I	232	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	I	233	THR
1	I	258	ARG
1	I	288	ASN
1	I	289	GLU
1	I	301	ILE
1	I	321	THR
1	I	338	MET
1	I	344	THR
1	I	351	THR
1	J	3	CYS
1	J	19	ILE
1	J	45	THR
1	J	105	ASN
1	J	116	SER
1	J	128	ILE
1	J	143	LEU
1	J	164	GLU
1	J	176	TYR
1	J	201	GLN
1	J	206	VAL
1	J	232	VAL
1	J	233	THR
1	J	258	ARG
1	J	288	ASN
1	J	289	GLU
1	J	301	ILE
1	J	321	THR
1	J	338	MET
1	J	344	THR
1	J	351	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	154	GLN
1	A	190	ASN
1	A	197	GLN
1	A	201	GLN
1	A	277	HIS
1	A	288	ASN
1	A	296	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	324	ASN
1	B	105	ASN
1	B	154	GLN
1	B	190	ASN
1	B	197	GLN
1	B	201	GLN
1	B	277	HIS
1	B	288	ASN
1	B	296	HIS
1	B	324	ASN
1	C	105	ASN
1	C	154	GLN
1	C	190	ASN
1	C	197	GLN
1	C	201	GLN
1	C	277	HIS
1	C	288	ASN
1	C	296	HIS
1	C	324	ASN
1	D	105	ASN
1	D	154	GLN
1	D	190	ASN
1	D	197	GLN
1	D	201	GLN
1	D	277	HIS
1	D	288	ASN
1	D	296	HIS
1	D	324	ASN
1	E	105	ASN
1	E	154	GLN
1	E	190	ASN
1	E	197	GLN
1	E	201	GLN
1	E	277	HIS
1	E	288	ASN
1	E	296	HIS
1	E	324	ASN
1	F	105	ASN
1	F	154	GLN
1	F	190	ASN
1	F	197	GLN
1	F	201	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	244	ASN
1	F	277	HIS
1	F	288	ASN
1	F	296	HIS
1	F	324	ASN
1	G	105	ASN
1	G	154	GLN
1	G	190	ASN
1	G	197	GLN
1	G	201	GLN
1	G	277	HIS
1	G	288	ASN
1	G	296	HIS
1	G	324	ASN
1	H	105	ASN
1	H	154	GLN
1	H	190	ASN
1	H	197	GLN
1	H	201	GLN
1	H	244	ASN
1	H	277	HIS
1	H	288	ASN
1	H	296	HIS
1	H	324	ASN
1	I	105	ASN
1	I	154	GLN
1	I	190	ASN
1	I	197	GLN
1	I	201	GLN
1	I	244	ASN
1	I	277	HIS
1	I	288	ASN
1	I	296	HIS
1	I	324	ASN
1	J	105	ASN
1	J	136	GLN
1	J	154	GLN
1	J	190	ASN
1	J	197	GLN
1	J	201	GLN
1	J	251	ASN
1	J	277	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	288	ASN
1	J	296	HIS
1	J	324	ASN

### 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 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 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
3	P3P	A	5001	2	14,14,14	3.91	4 (28%)	19,21,21	1.77	5 (26%)
4	ADP	A	6001	2	29,29,29	1.16	2 (6%)	45,45,45	3.21	13 (28%)
3	P3P	B	5002	1,2	14,14,14	2.84	6 (42%)	19,21,21	2.51	8 (42%)
4	ADP	B	6002	2	29,29,29	1.23	3 (10%)	45,45,45	3.31	15 (33%)
3	P3P	C	5003	2	14,14,14	3.57	4 (28%)	19,21,21	2.82	10 (52%)
4	ADP	C	6003	2	29,29,29	1.19	3 (10%)	45,45,45	2.73	11 (24%)
3	P3P	D	5004	2	14,14,14	4.12	4 (28%)	19,21,21	1.57	4 (21%)
4	ADP	D	6005	2	29,29,29	1.12	2 (6%)	45,45,45	2.62	14 (31%)
3	P3P	E	5005	2	14,14,14	2.47	4 (28%)	19,21,21	2.19	5 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ADP	E	6004	2	29,29,29	1.25	4 (13%)	45,45,45	2.50	14 (31%)
3	P3P	F	5007	2	14,14,14	2.74	3 (21%)	19,21,21	1.83	4 (21%)
4	ADP	F	6007	2	29,29,29	1.06	1 (3%)	45,45,45	2.86	11 (24%)
3	P3P	G	5006	2	14,14,14	3.86	4 (28%)	19,21,21	1.55	5 (26%)
4	ADP	G	6006	2	29,29,29	0.96	2 (6%)	45,45,45	2.11	11 (24%)
3	P3P	H	5010	2	14,14,14	4.50	5 (35%)	19,21,21	2.16	4 (21%)
4	ADP	H	6010	2	29,29,29	1.61	3 (10%)	45,45,45	2.62	16 (35%)
3	P3P	I	5008	2	14,14,14	3.57	5 (35%)	19,21,21	3.07	5 (26%)
4	ADP	I	6008	2	29,29,29	1.04	1 (3%)	45,45,45	2.80	17 (37%)
3	P3P	J	5009	2	14,14,14	3.05	3 (21%)	19,21,21	2.30	5 (26%)
4	ADP	J	6009	2	29,29,29	1.05	2 (6%)	45,45,45	2.75	9 (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
3	P3P	A	5001	2	-	1/14/16/16	0/0/0/0
4	ADP	A	6001	2	-	1/16/32/32	0/1/3/3
3	P3P	B	5002	1,2	-	0/14/16/16	0/0/0/0
4	ADP	B	6002	2	-	0/16/32/32	0/1/3/3
3	P3P	C	5003	2	-	0/14/16/16	0/0/0/0
4	ADP	C	6003	2	-	0/16/32/32	0/1/3/3
3	P3P	D	5004	2	-	0/14/16/16	0/0/0/0
4	ADP	D	6005	2	-	0/16/32/32	0/1/3/3
3	P3P	E	5005	2	-	0/14/16/16	0/0/0/0
4	ADP	E	6004	2	-	0/16/32/32	0/1/3/3
3	P3P	F	5007	2	-	1/14/16/16	0/0/0/0
4	ADP	F	6007	2	-	0/16/32/32	0/1/3/3
3	P3P	G	5006	2	-	0/14/16/16	0/0/0/0
4	ADP	G	6006	2	-	0/16/32/32	0/1/3/3
3	P3P	H	5010	2	-	0/14/16/16	0/0/0/0
4	ADP	H	6010	2	-	0/16/32/32	0/1/3/3
3	P3P	I	5008	2	-	1/14/16/16	0/0/0/0
4	ADP	I	6008	2	-	0/16/32/32	0/1/3/3
3	P3P	J	5009	2	-	0/14/16/16	0/0/0/0
4	ADP	J	6009	2	-	0/16/32/32	0/1/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5010	P3P	PDP-CGP	-13.57	1.67	1.79
3	A	5001	P3P	PDP-CGP	-11.69	1.69	1.79
3	I	5008	P3P	PDP-CGP	-10.28	1.70	1.79
3	G	5006	P3P	PDP-CGP	-10.10	1.70	1.79
3	D	5004	P3P	PDP-CGP	-9.91	1.70	1.79
3	C	5003	P3P	PDP-CGP	-9.87	1.70	1.79
3	J	5009	P3P	PDP-CGP	-8.67	1.71	1.79
3	D	5004	P3P	PDP-CEP	-8.39	1.69	1.78
3	G	5006	P3P	PDP-CEP	-8.10	1.69	1.78
3	B	5002	P3P	PDP-CGP	-7.49	1.73	1.79
3	H	5010	P3P	PDP-CEP	-7.39	1.70	1.78
3	F	5007	P3P	PDP-CGP	-7.10	1.73	1.79
3	C	5003	P3P	PDP-CEP	-6.88	1.70	1.78
3	A	5001	P3P	PDP-OEA	5.86	1.61	1.49
3	J	5009	P3P	PDP-CEP	-5.63	1.72	1.78
3	D	5004	P3P	PDP-OEA	5.62	1.61	1.49
3	F	5007	P3P	PDP-CEP	-5.38	1.72	1.78
3	I	5008	P3P	CBP-CGP	-5.36	1.50	1.53
4	H	6010	ADP	C2'-C1'	-5.31	1.45	1.53
3	D	5004	P3P	CBP-CGP	-5.21	1.50	1.53
3	E	5005	P3P	PDP-OEA	5.07	1.60	1.49
3	E	5005	P3P	PDP-CEP	-5.03	1.72	1.78
3	C	5003	P3P	PDP-OEA	4.91	1.59	1.49
3	F	5007	P3P	PDP-OEA	4.48	1.58	1.49
3	A	5001	P3P	PDP-CEP	-4.43	1.73	1.78
3	G	5006	P3P	CBP-CGP	-4.31	1.50	1.53
3	B	5002	P3P	PDP-CEP	-4.25	1.73	1.78
3	I	5008	P3P	PDP-OEA	4.24	1.58	1.49
3	E	5005	P3P	PDP-CGP	-4.22	1.75	1.79
3	A	5001	P3P	CBP-CGP	-4.12	1.50	1.53
3	H	5010	P3P	PDP-OEA	4.03	1.57	1.49
4	H	6010	ADP	C4-N9	-4.02	1.31	1.37
3	G	5006	P3P	PDP-OEA	4.01	1.57	1.49
3	J	5009	P3P	PDP-OEA	3.93	1.57	1.49
3	H	5010	P3P	OP-CP	3.51	1.34	1.22
3	I	5008	P3P	PDP-CEP	-3.43	1.74	1.78
4	I	6008	ADP	O4'-C1'	3.29	1.46	1.41
4	A	6001	ADP	C4-N3	3.07	1.40	1.35
3	B	5002	P3P	PDP-OEA	3.06	1.55	1.49
4	C	6003	ADP	C2-N3	3.05	1.38	1.32
3	H	5010	P3P	CBP-CGP	-3.06	1.51	1.53
3	B	5002	P3P	P12-OEB	2.89	1.65	1.60
4	B	6002	ADP	O4'-C1'	2.77	1.45	1.41

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	6002	ADP	C4-N3	2.74	1.39	1.35
4	E	6004	ADP	O4'-C1'	2.74	1.45	1.41
3	E	5005	P3P	P12-O13	2.68	1.64	1.54
4	G	6006	ADP	O4'-C1'	2.66	1.45	1.41
4	F	6007	ADP	PA-O3A	2.65	1.64	1.59
4	C	6003	ADP	O4'-C1'	2.54	1.45	1.41
3	B	5002	P3P	P12-O15	2.53	1.59	1.51
3	I	5008	P3P	P12-OEB	2.52	1.64	1.60
3	B	5002	P3P	OP-CP	2.50	1.30	1.22
4	D	6005	ADP	PA-O3A	2.45	1.64	1.59
4	H	6010	ADP	C8-N9	-2.36	1.33	1.36
4	B	6002	ADP	PB-O3A	2.36	1.64	1.60
3	C	5003	P3P	CBP-CGP	-2.35	1.51	1.53
4	D	6005	ADP	C2'-C3'	-2.33	1.46	1.53
4	J	6009	ADP	C4-N9	-2.31	1.34	1.37
4	A	6001	ADP	C2'-C3'	-2.18	1.47	1.53
4	E	6004	ADP	PB-O3A	2.07	1.63	1.60
4	J	6009	ADP	C2'-C1'	-2.06	1.50	1.53
4	E	6004	ADP	C2'-C1'	2.04	1.56	1.53
4	C	6003	ADP	C4-N9	-2.03	1.34	1.37
4	E	6004	ADP	PA-O3A	2.03	1.63	1.59
4	G	6006	ADP	C4-N9	-2.01	1.34	1.37

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6002	ADP	N3-C2-N1	-14.87	116.28	128.71
4	J	6009	ADP	O4'-C1'-N9	12.79	120.33	108.44
4	A	6001	ADP	N3-C2-N1	-12.09	118.60	128.71
4	A	6001	ADP	O4'-C1'-N9	11.32	118.97	108.44
4	F	6007	ADP	O4'-C1'-N9	10.89	118.57	108.44
3	I	5008	P3P	CP-CAP-NP	10.54	126.81	109.36
4	F	6007	ADP	N3-C2-N1	-10.29	120.11	128.71
4	C	6003	ADP	O4'-C1'-N9	10.26	117.98	108.44
4	H	6010	ADP	N3-C2-N1	-10.20	120.19	128.71
4	B	6002	ADP	O4'-C1'-N9	10.00	117.75	108.44
4	I	6008	ADP	N3-C2-N1	-9.97	120.38	128.71
4	D	6005	ADP	N3-C2-N1	-9.20	121.02	128.71
4	G	6006	ADP	N3-C2-N1	-9.07	121.12	128.71
4	C	6003	ADP	N3-C2-N1	-8.73	121.41	128.71
4	E	6004	ADP	N3-C2-N1	-8.21	121.84	128.71
4	E	6004	ADP	O4'-C1'-N9	8.03	115.91	108.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	6008	ADP	C3'-C2'-C1'	-7.92	88.50	100.91
4	J	6009	ADP	N3-C2-N1	-7.35	122.56	128.71
3	H	5010	P3P	CP-CAP-NP	7.31	121.47	109.36
4	I	6008	ADP	O4'-C1'-N9	6.78	114.75	108.44
4	A	6001	ADP	N3-C4-N9	6.76	137.64	125.43
3	C	5003	P3P	CP-CAP-NP	6.63	120.34	109.36
3	J	5009	P3P	PDP-CGP-CBP	6.54	124.57	114.87
4	B	6002	ADP	N3-C4-N9	6.27	136.75	125.43
4	F	6007	ADP	C3'-C2'-C1'	-5.95	91.60	100.91
3	E	5005	P3P	PDP-CGP-CBP	5.80	123.48	114.87
4	D	6005	ADP	C3'-C2'-C1'	-5.61	92.13	100.91
4	H	6010	ADP	O2'-C2'-C1'	-5.60	94.29	111.23
3	B	5002	P3P	CP-CAP-NP	5.37	118.25	109.36
4	D	6005	ADP	O4'-C1'-N9	5.30	113.37	108.44
4	D	6005	ADP	C4'-O4'-C1'	-5.26	104.03	109.75
4	E	6004	ADP	C3'-C2'-C1'	-5.22	92.74	100.91
3	I	5008	P3P	OTP-CP-OP	-5.17	112.37	124.07
4	H	6010	ADP	C8-N9-C4	4.95	110.67	106.90
4	C	6003	ADP	O3'-C3'-C2'	-4.90	95.90	111.83
4	G	6006	ADP	O4'-C1'-N9	4.78	112.89	108.44
4	D	6005	ADP	C8-N9-C4	4.70	110.48	106.90
4	I	6008	ADP	C8-N9-C4	4.52	110.35	106.90
4	A	6001	ADP	C5-C4-N3	-4.44	116.03	125.70
4	I	6008	ADP	N3-C4-N9	4.41	133.39	125.43
4	J	6009	ADP	O4'-C1'-C2'	-4.34	100.12	106.77
4	F	6007	ADP	C4'-O4'-C1'	-4.23	105.16	109.75
4	E	6004	ADP	O3B-PB-O1B	4.22	124.24	110.44
4	E	6004	ADP	N3-C4-N9	4.13	132.89	125.43
3	B	5002	P3P	O13-P12-O15	4.09	123.80	110.44
4	G	6006	ADP	N3-C4-N9	4.08	132.81	125.43
4	C	6003	ADP	N3-C4-N9	4.06	132.77	125.43
3	A	5001	P3P	CP-CAP-NP	3.93	115.86	109.36
4	D	6005	ADP	C1'-N9-C4	-3.90	119.90	126.64
4	F	6007	ADP	N3-C4-N9	3.87	132.42	125.43
4	D	6005	ADP	C4-C5-N7	-3.83	106.24	109.52
3	F	5007	P3P	CEP-PDP-CGP	3.82	116.51	107.36
3	E	5005	P3P	O14-P12-O13	3.82	122.49	107.61
4	J	6009	ADP	C4-C5-N7	-3.79	106.28	109.52
4	A	6001	ADP	C2-N3-C4	3.78	124.78	114.01
4	C	6003	ADP	C5-C4-N3	-3.74	117.55	125.70
3	C	5003	P3P	PDP-CGP-CBP	3.73	120.41	114.87
4	A	6001	ADP	C5-C6-N6	-3.72	112.30	120.72

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6010	ADP	O3B-PB-O1B	3.69	122.49	110.44
3	C	5003	P3P	OTP-CP-OP	-3.66	115.79	124.07
4	H	6010	ADP	C1'-N9-C4	-3.65	120.32	126.64
4	B	6002	ADP	C4'-O4'-C1'	-3.65	105.78	109.75
3	C	5003	P3P	O14-P12-O13	3.63	121.74	107.61
4	A	6001	ADP	O3'-C3'-C2'	-3.62	100.06	111.83
4	C	6003	ADP	C2'-C3'-C4'	3.58	109.79	102.65
3	F	5007	P3P	OEA-PDP-CEP	-3.58	103.42	111.49
3	B	5002	P3P	OP-CP-CAP	3.56	128.63	118.36
3	B	5002	P3P	OEA-PDP-CEP	-3.55	103.48	111.49
3	C	5003	P3P	OEA-PDP-CEP	-3.55	103.49	111.49
4	J	6009	ADP	N3-C4-N9	3.54	131.83	125.43
3	E	5005	P3P	OEB-PDP-CGP	3.53	117.22	106.94
3	J	5009	P3P	CP-CAP-NP	3.52	115.20	109.36
4	D	6005	ADP	O3'-C3'-C2'	-3.51	100.42	111.83
4	B	6002	ADP	C2-N3-C4	3.50	123.96	114.01
4	B	6002	ADP	C5-C6-N6	-3.49	112.82	120.72
4	F	6007	ADP	O2'-C2'-C1'	3.48	121.77	111.23
4	J	6009	ADP	C5-C4-N3	-3.46	118.17	125.70
3	B	5002	P3P	PDP-CGP-CBP	3.44	119.97	114.87
4	A	6001	ADP	O2'-C2'-C3'	-3.41	100.76	111.83
4	B	6002	ADP	C5-C4-N3	-3.39	118.32	125.70
4	D	6005	ADP	N3-C4-N9	3.38	131.53	125.43
3	J	5009	P3P	OTP-CP-OP	-3.37	116.44	124.07
4	H	6010	ADP	N3-C4-N9	3.35	131.49	125.43
4	I	6008	ADP	C1'-N9-C4	-3.33	120.87	126.64
4	B	6002	ADP	N6-C6-N1	3.31	125.87	119.36
3	C	5003	P3P	OTP-CP-CAP	3.31	124.30	116.88
3	D	5004	P3P	O14-P12-O15	3.26	121.10	110.44
4	C	6003	ADP	C4-C5-N7	-3.25	106.74	109.52
4	C	6003	ADP	C2-N3-C4	3.23	123.20	114.01
4	B	6002	ADP	PA-O3A-PB	-3.20	122.31	131.68
4	B	6002	ADP	C2'-C1'-N9	-3.19	105.07	113.27
3	G	5006	P3P	OEA-PDP-CEP	-3.18	104.32	111.49
3	E	5005	P3P	CP-CAP-NP	3.09	114.49	109.36
4	I	6008	ADP	C4'-O4'-C1'	-3.04	106.45	109.75
3	J	5009	P3P	O14-P12-O13	3.02	119.38	107.61
3	B	5002	P3P	O14-P12-O15	-2.98	100.71	110.44
4	A	6001	ADP	O5'-PA-O1A	-2.95	97.83	109.37
4	E	6004	ADP	O2'-C2'-C1'	2.93	120.09	111.23
3	I	5008	P3P	O14-P12-O13	2.92	118.99	107.61
4	J	6009	ADP	O3B-PB-O1B	2.91	119.96	110.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6001	ADP	O2B-PB-O1B	2.90	119.93	110.44
4	H	6010	ADP	O3'-C3'-C2'	-2.90	102.40	111.83
4	G	6006	ADP	C5-C4-N3	-2.88	119.43	125.70
4	G	6006	ADP	O3B-PB-O1B	2.87	119.83	110.44
3	G	5006	P3P	CP-CAP-NP	2.81	114.02	109.36
4	H	6010	ADP	C2'-C3'-C4'	2.81	108.25	102.65
4	B	6002	ADP	C8-N9-C4	2.81	109.04	106.90
3	A	5001	P3P	O14-P12-O13	2.80	118.51	107.61
4	H	6010	ADP	O4'-C1'-N9	2.79	111.04	108.44
4	C	6003	ADP	PA-O3A-PB	-2.78	123.53	131.68
3	F	5007	P3P	OTP-CP-OP	-2.77	117.81	124.07
4	E	6004	ADP	O3'-C3'-C4'	-2.76	102.94	111.08
3	D	5004	P3P	CP-CAP-NP	2.76	113.93	109.36
3	C	5003	P3P	OEA-PDP-CGP	2.76	119.46	110.71
4	I	6008	ADP	N7-C8-N9	-2.71	106.69	114.36
4	A	6001	ADP	C4'-O4'-C1'	-2.69	106.82	109.75
3	A	5001	P3P	CGP-CBP-CAP	-2.69	106.07	113.66
3	C	5003	P3P	O14-P12-O15	2.69	119.24	110.44
3	B	5002	P3P	OTP-CP-OP	-2.68	118.01	124.07
4	I	6008	ADP	O5'-C5'-C4'	2.65	118.67	108.94
3	A	5001	P3P	OEA-PDP-CGP	-2.64	102.32	110.71
4	E	6004	ADP	C2'-C1'-N9	2.64	120.05	113.27
4	H	6010	ADP	O3B-PB-O2B	2.62	117.82	107.61
4	E	6004	ADP	O3'-C3'-C2'	-2.61	103.33	111.83
3	I	5008	P3P	OTP-CP-CAP	2.61	122.73	116.88
4	F	6007	ADP	C1'-N9-C4	-2.61	122.13	126.64
3	F	5007	P3P	O14-P12-O13	2.60	117.75	107.61
3	D	5004	P3P	O14-P12-O13	2.59	117.71	107.61
4	J	6009	ADP	C3'-C2'-C1'	-2.59	96.86	100.91
4	E	6004	ADP	C5-C4-N3	-2.59	120.07	125.70
4	G	6006	ADP	C3'-C2'-C1'	-2.56	96.90	100.91
4	I	6008	ADP	C2'-C1'-N9	2.56	119.84	113.27
4	D	6005	ADP	N7-C8-N9	-2.55	107.15	114.36
4	I	6008	ADP	O2'-C2'-C1'	2.55	118.93	111.23
4	I	6008	ADP	O2B-PB-O1B	2.55	118.76	110.44
3	B	5002	P3P	CEP-PDP-CGP	2.52	113.38	107.36
4	H	6010	ADP	C4-C5-N7	-2.51	107.37	109.52
3	H	5010	P3P	OTP-CP-CAP	-2.50	111.28	116.88
4	H	6010	ADP	C2'-C1'-N9	-2.50	106.86	113.27
4	H	6010	ADP	O2B-PB-O1B	-2.49	102.29	110.44
4	C	6003	ADP	O3'-C3'-C4'	-2.49	103.74	111.08
4	I	6008	ADP	O3A-PB-O1B	-2.47	94.11	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6005	ADP	O3B-PB-O2B	2.46	117.19	107.61
3	G	5006	P3P	O13-P12-O15	2.45	118.46	110.44
4	H	6010	ADP	O3A-PA-O5'	-2.44	92.49	103.41
4	I	6008	ADP	C5-C4-N3	-2.43	120.41	125.70
4	H	6010	ADP	PA-O3A-PB	-2.43	124.56	131.68
4	F	6007	ADP	C5-C4-N3	-2.41	120.45	125.70
4	F	6007	ADP	C2'-C1'-N9	2.41	119.45	113.27
4	E	6004	ADP	C2'-C3'-C4'	2.38	107.39	102.65
4	F	6007	ADP	O2B-PB-O1B	2.37	118.20	110.44
3	E	5005	P3P	OTP-CP-OP	-2.34	118.77	124.07
3	G	5006	P3P	OEB-P12-O15	-2.34	95.00	111.00
3	H	5010	P3P	O13-P12-OEB	2.33	116.20	105.14
4	G	6006	ADP	C2-N3-C4	2.32	120.62	114.01
3	C	5003	P3P	O13-P12-O15	-2.32	102.86	110.44
4	H	6010	ADP	N7-C8-N9	-2.31	107.83	114.36
3	C	5003	P3P	O13-P12-OEB	2.30	116.05	105.14
4	A	6001	ADP	O3A-PB-O1B	-2.30	95.29	111.00
4	F	6007	ADP	C2-N3-C4	2.29	120.52	114.01
4	J	6009	ADP	C2-N3-C4	2.28	120.50	114.01
3	D	5004	P3P	OEB-P12-O15	-2.27	95.48	111.00
4	G	6006	ADP	O3'-C3'-C2'	-2.25	104.51	111.83
4	D	6005	ADP	C2-N3-C4	2.25	120.41	114.01
3	A	5001	P3P	OEB-PDP-CEP	2.23	115.06	105.89
4	B	6002	ADP	O3'-C3'-C2'	-2.23	104.57	111.83
3	H	5010	P3P	OEB-PDP-CGP	2.22	113.39	106.94
4	B	6002	ADP	O3B-PB-O1B	2.21	117.66	110.44
4	G	6006	ADP	O2'-C2'-C1'	2.20	117.89	111.23
3	J	5009	P3P	OP-CP-CAP	2.20	124.71	118.36
3	I	5008	P3P	OP-CP-CAP	2.20	124.70	118.36
4	I	6008	ADP	O4'-C4'-C3'	-2.20	100.72	105.17
4	I	6008	ADP	C2-N3-C4	2.18	120.20	114.01
4	E	6004	ADP	N6-C6-N1	2.17	123.62	119.36
3	G	5006	P3P	CEP-PDP-CGP	2.15	112.51	107.36
4	B	6002	ADP	C3'-C2'-C1'	-2.13	97.58	100.91
4	C	6003	ADP	O3A-PA-O5'	-2.09	94.04	103.41
4	D	6005	ADP	C5-C4-N3	-2.09	121.14	125.70
4	E	6004	ADP	O5'-C5'-C4'	-2.08	101.31	108.94
4	D	6005	ADP	O4'-C1'-C2'	2.08	109.95	106.77
4	A	6001	ADP	C2'-C3'-C4'	2.05	106.74	102.65
4	E	6004	ADP	O2'-C2'-C3'	-2.05	105.15	111.83
4	G	6006	ADP	PA-O3A-PB	-2.05	125.67	131.68
4	G	6006	ADP	C2'-C1'-N9	2.04	118.50	113.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	6008	ADP	O3B-PB-O1B	2.03	117.07	110.44
4	B	6002	ADP	N7-C8-N9	-2.01	108.69	114.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	5008	P3P	CEP-PDP-OEB-P12
3	A	5001	P3P	CEP-PDP-OEB-P12
3	F	5007	P3P	CEP-PDP-OEB-P12
4	A	6001	ADP	C2'-C1'-N9-C8

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	353/356 (99%)	-0.39	0 100 100	49, 66, 89, 100	0
1	B	353/356 (99%)	-0.36	0 100 100	49, 66, 89, 100	0
1	C	353/356 (99%)	-0.38	0 100 100	49, 66, 89, 100	0
1	D	353/356 (99%)	-0.37	0 100 100	49, 67, 89, 100	0
1	E	353/356 (99%)	-0.38	0 100 100	49, 67, 89, 100	0
1	F	353/356 (99%)	-0.37	0 100 100	49, 67, 89, 100	0
1	G	353/356 (99%)	-0.37	0 100 100	49, 67, 89, 100	0
1	H	353/356 (99%)	-0.36	0 100 100	49, 66, 89, 100	0
1	I	353/356 (99%)	-0.38	0 100 100	49, 66, 89, 100	0
1	J	353/356 (99%)	-0.36	0 100 100	49, 66, 89, 100	0
All	All	3530/3560 (99%)	-0.37	0 100 100	49, 67, 89, 100	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MN	F	1051	1/1	0.24	2.23	86,86,86,86	0
4	ADP	A	6001	27/27	0.24	1.64	55,76,90,90	0
4	ADP	C	6003	27/27	0.25	1.38	45,68,81,83	0
2	MN	C	1021	1/1	0.26	1.34	88,88,88,88	0
4	ADP	E	6004	27/27	0.25	0.94	81,87,94,95	0
3	P3P	C	5003	15/15	0.20	0.74	48,53,58,59	0
2	MN	A	1001	1/1	0.23	0.72	52,52,52,52	0
4	ADP	D	6005	27/27	0.22	0.53	67,73,90,90	0
3	P3P	A	5001	15/15	0.18	0.28	50,54,64,65	0
3	P3P	D	5004	15/15	0.20	0.24	64,67,75,76	0
3	P3P	F	5007	15/15	0.20	0.15	66,68,73,77	0
3	P3P	J	5009	15/15	0.21	0.13	46,48,56,58	0
3	P3P	G	5006	15/15	0.18	0.04	61,67,80,80	0
4	ADP	F	6007	27/27	0.20	-0.05	76,85,92,92	0
4	ADP	J	6009	27/27	0.21	-0.10	44,54,60,62	0
4	ADP	G	6006	27/27	0.19	-0.10	55,68,76,79	0
3	P3P	E	5005	15/15	0.19	-0.12	65,73,78,81	0
4	ADP	I	6008	27/27	0.17	-0.16	62,71,74,75	0
3	P3P	I	5008	15/15	0.18	-0.21	41,49,59,59	0
3	P3P	B	5002	15/15	0.18	-0.25	30,32,40,41	0
2	MN	B	1011	1/1	0.20	-0.31	61,61,61,61	0
2	MN	F	1053	1/1	0.17	-0.35	63,63,63,63	0
4	ADP	B	6002	27/27	0.16	-0.44	37,46,53,54	0
2	MN	B	1013	1/1	0.18	-0.59	54,54,54,54	0
4	ADP	H	6010	27/27	0.16	-0.62	29,31,40,43	0
2	MN	D	1032	1/1	0.20	-0.67	83,83,83,83	0
2	MN	D	1033	1/1	0.15	-0.73	51,51,51,51	0
3	P3P	H	5010	15/15	0.15	-0.75	30,35,41,41	0
2	MN	A	1002	1/1	0.19	-0.84	62,62,62,62	0
2	MN	J	1091	1/1	0.21	-0.96	52,52,52,52	0
2	MN	C	1023	1/1	0.15	-1.14	56,56,56,56	0
2	MN	G	1062	1/1	0.18	-1.19	69,69,69,69	0
2	MN	H	1071	1/1	0.16	-1.30	52,52,52,52	0
2	MN	D	1031	1/1	0.14	-1.43	57,57,57,57	0
2	MN	F	1052	1/1	0.15	-1.49	54,54,54,54	0
2	MN	I	1081	1/1	0.14	-1.51	53,53,53,53	0
2	MN	I	1082	1/1	0.14	-1.51	67,67,67,67	0
2	MN	E	1043	1/1	0.14	-1.61	71,71,71,71	0
2	MN	C	1022	1/1	0.14	-1.61	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	J	1093	1/1	0.15	-1.68	41,41,41,41	0
2	MN	J	1092	1/1	0.19	-1.69	61,61,61,61	0
2	MN	E	1042	1/1	0.18	-1.81	73,73,73,73	0
2	MN	I	1083	1/1	0.11	-1.87	64,64,64,64	0
2	MN	G	1063	1/1	0.14	-1.91	51,51,51,51	0
2	MN	A	1003	1/1	0.12	-2.01	40,40,40,40	0
2	MN	H	1073	1/1	0.11	-2.08	28,28,28,28	0
2	MN	B	1012	1/1	0.13	-2.17	32,32,32,32	0
2	MN	H	1072	1/1	0.14	-3.90	49,49,49,49	0
2	MN	G	1061	1/1	0.16	-4.07	58,58,58,58	0
2	MN	E	1041	1/1	0.16	-4.80	68,68,68,68	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.