



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:39 PM BST

PDB ID : 5BP0  
Title : X-ray crystal structure of Lymnaea stagnalis acetylcholine binding protein (Ls-AChBP) in complex with 5-Fluoronicotine (TI-4650)  
Authors : Bobango, J.; Sankaran, B.; Park, J.F.; Wu, J.; Talley, T.T.  
Deposited on : 2015-05-27  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

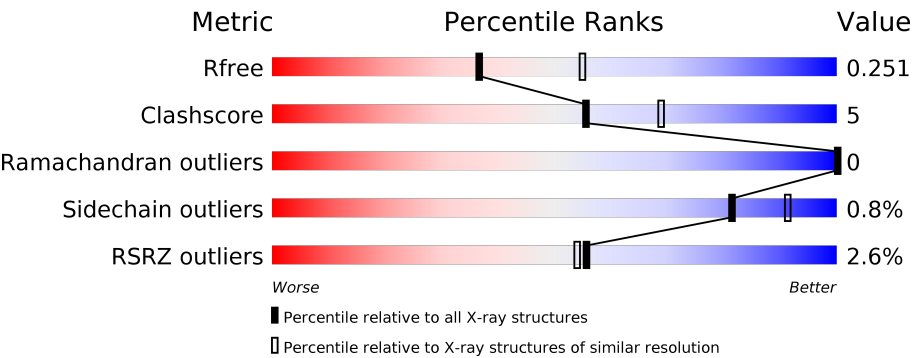
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div><div>%</div><div><div></div><div>85%</div><div>6%</div><div>9%</div></div></div>
1	B	218	<div><div>%</div><div><div></div><div>87%</div><div>7%</div><div>6%</div></div></div>
1	C	218	<div><div></div><div><div></div><div>88%</div><div>7%</div><div>5%</div></div></div>
1	D	218	<div><div>%</div><div><div></div><div>86%</div><div>9%</div><div>5%</div></div></div>
1	E	218	<div><div>2%</div><div><div></div><div>81%</div><div>11%</div><div>7%</div></div></div>
1	F	218	<div><div>4%</div><div><div></div><div>77%</div><div>12%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	218	
1	H	218	
1	I	218	
1	J	218	

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
3	FN1	D	302	-	-	X	-
3	FN1	J	303	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30290 atoms, of which 14369 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	199	Total	C	H	N	O	S	0	0	0
			2934	958	1421	251	299	5			
1	B	205	Total	C	H	N	O	S	0	0	0
			3067	997	1482	257	326	5			
1	C	208	Total	C	H	N	O	S	0	0	0
			3004	992	1428	252	327	5			
1	D	207	Total	C	H	N	O	S	0	0	0
			3107	1005	1503	265	329	5			
1	E	202	Total	C	H	N	O	S	0	0	0
			2940	966	1403	254	312	5			
1	F	193	Total	C	H	N	O	S	0	0	0
			2708	900	1293	235	277	3			
1	G	201	Total	C	H	N	O	S	0	0	0
			2980	972	1438	254	311	5			
1	H	201	Total	C	H	N	O	S	0	0	0
			3090	991	1508	272	314	5			
1	I	203	Total	C	H	N	O	S	0	0	0
			3021	984	1452	259	321	5			
1	J	203	Total	C	H	N	O	S	0	0	0
			2816	939	1329	243	300	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P58154
A	-6	TYR	-	expression tag	UNP P58154
A	-5	LYS	-	expression tag	UNP P58154
A	-4	ASP	-	expression tag	UNP P58154
A	-3	ASP	-	expression tag	UNP P58154
A	-2	ASP	-	expression tag	UNP P58154
A	-1	ASP	-	expression tag	UNP P58154
A	0	LYS	-	expression tag	UNP P58154
B	-7	ASP	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP P58154
B	-5	LYS	-	expression tag	UNP P58154
B	-4	ASP	-	expression tag	UNP P58154
B	-3	ASP	-	expression tag	UNP P58154
B	-2	ASP	-	expression tag	UNP P58154
B	-1	ASP	-	expression tag	UNP P58154
B	0	LYS	-	expression tag	UNP P58154
C	-7	ASP	-	expression tag	UNP P58154
C	-6	TYR	-	expression tag	UNP P58154
C	-5	LYS	-	expression tag	UNP P58154
C	-4	ASP	-	expression tag	UNP P58154
C	-3	ASP	-	expression tag	UNP P58154
C	-2	ASP	-	expression tag	UNP P58154
C	-1	ASP	-	expression tag	UNP P58154
C	0	LYS	-	expression tag	UNP P58154
D	-7	ASP	-	expression tag	UNP P58154
D	-6	TYR	-	expression tag	UNP P58154
D	-5	LYS	-	expression tag	UNP P58154
D	-4	ASP	-	expression tag	UNP P58154
D	-3	ASP	-	expression tag	UNP P58154
D	-2	ASP	-	expression tag	UNP P58154
D	-1	ASP	-	expression tag	UNP P58154
D	0	LYS	-	expression tag	UNP P58154
E	-7	ASP	-	expression tag	UNP P58154
E	-6	TYR	-	expression tag	UNP P58154
E	-5	LYS	-	expression tag	UNP P58154
E	-4	ASP	-	expression tag	UNP P58154
E	-3	ASP	-	expression tag	UNP P58154
E	-2	ASP	-	expression tag	UNP P58154
E	-1	ASP	-	expression tag	UNP P58154
E	0	LYS	-	expression tag	UNP P58154
F	-7	ASP	-	expression tag	UNP P58154
F	-6	TYR	-	expression tag	UNP P58154
F	-5	LYS	-	expression tag	UNP P58154
F	-4	ASP	-	expression tag	UNP P58154
F	-3	ASP	-	expression tag	UNP P58154
F	-2	ASP	-	expression tag	UNP P58154
F	-1	ASP	-	expression tag	UNP P58154
F	0	LYS	-	expression tag	UNP P58154
G	-7	ASP	-	expression tag	UNP P58154
G	-6	TYR	-	expression tag	UNP P58154
G	-5	LYS	-	expression tag	UNP P58154

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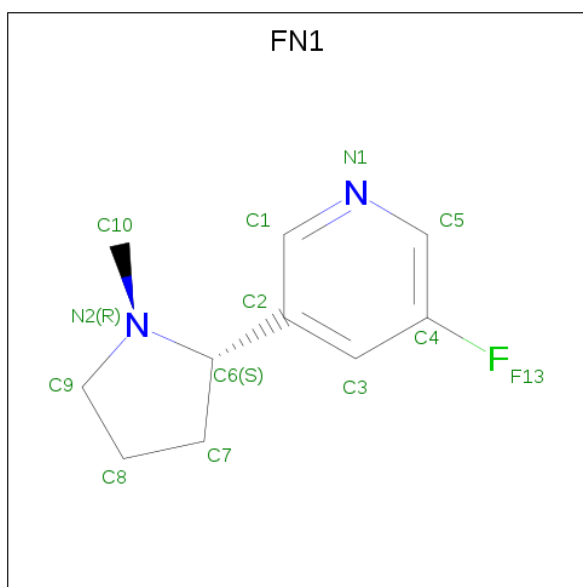
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
H	-5	LYS	-	expression tag	UNP P58154
H	-4	ASP	-	expression tag	UNP P58154
H	-3	ASP	-	expression tag	UNP P58154
H	-2	ASP	-	expression tag	UNP P58154
H	-1	ASP	-	expression tag	UNP P58154
H	0	LYS	-	expression tag	UNP P58154
I	-7	ASP	-	expression tag	UNP P58154
I	-6	TYR	-	expression tag	UNP P58154
I	-5	LYS	-	expression tag	UNP P58154
I	-4	ASP	-	expression tag	UNP P58154
I	-3	ASP	-	expression tag	UNP P58154
I	-2	ASP	-	expression tag	UNP P58154
I	-1	ASP	-	expression tag	UNP P58154
I	0	LYS	-	expression tag	UNP P58154
J	-7	ASP	-	expression tag	UNP P58154
J	-6	TYR	-	expression tag	UNP P58154
J	-5	LYS	-	expression tag	UNP P58154
J	-4	ASP	-	expression tag	UNP P58154
J	-3	ASP	-	expression tag	UNP P58154
J	-2	ASP	-	expression tag	UNP P58154
J	-1	ASP	-	expression tag	UNP P58154
J	0	LYS	-	expression tag	UNP P58154

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

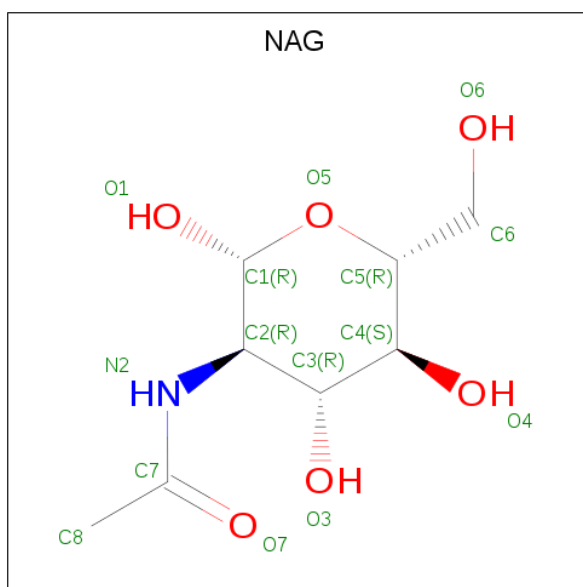
- Molecule 3 is 5-fluoronicotine (three-letter code: FN1) (formula: C<sub>10</sub>H<sub>13</sub>FN<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	B	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	C	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	D	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	E	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	F	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	H	1	Total	C	F	H	N	0	0
			27	10	1	14	2		
3	J	1	Total	C	F	H	N	0	0
			27	10	1	14	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

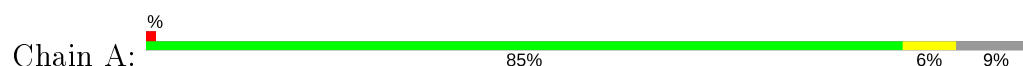
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	46	Total	O	0	0
			46	46		
5	C	43	Total	O	0	0
			43	43		
5	D	46	Total	O	0	0
			46	46		
5	E	28	Total	O	0	0
			28	28		
5	F	16	Total	O	0	0
			16	16		
5	G	29	Total	O	0	0
			29	29		
5	H	32	Total	O	0	0
			32	32		
5	I	37	Total	O	0	0
			37	37		
5	J	26	Total	O	0	0
			26	26		

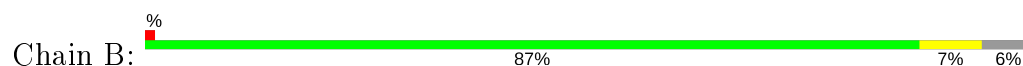
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acetylcholine-binding protein



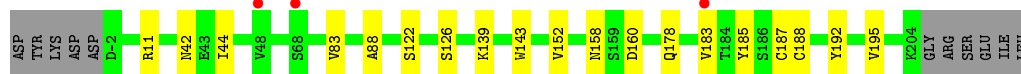
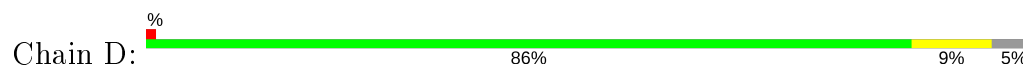
- Molecule 1: Acetylcholine-binding protein



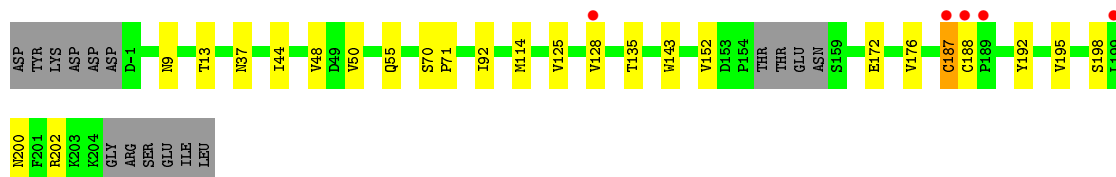
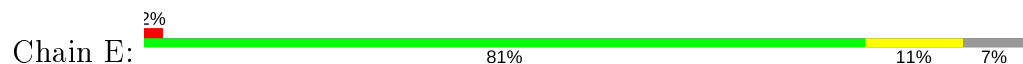
- Molecule 1: Acetylcholine-binding protein



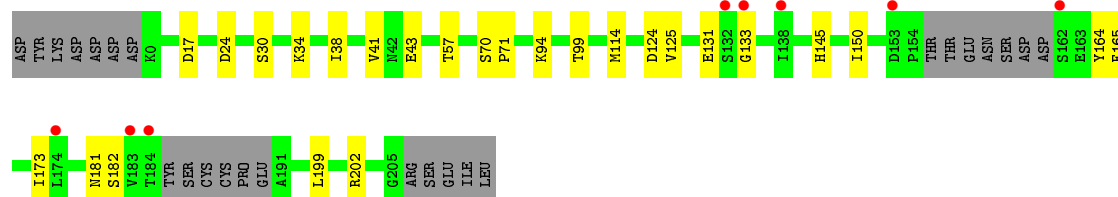
- Molecule 1: Acetylcholine-binding protein



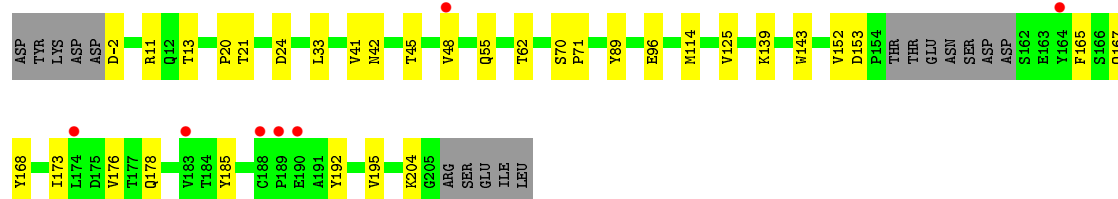
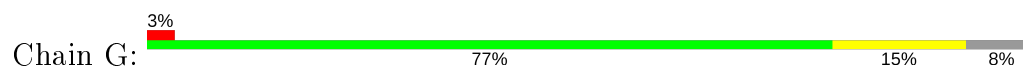
- Molecule 1: Acetylcholine-binding protein



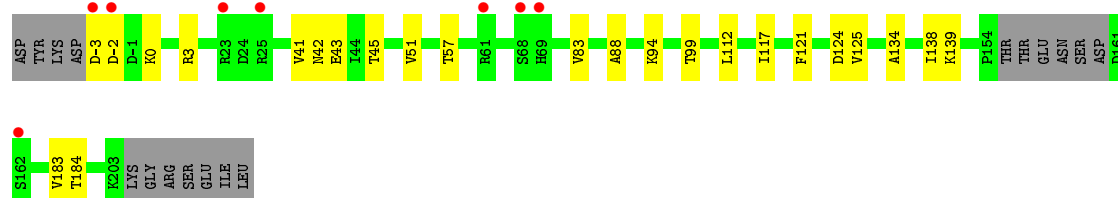
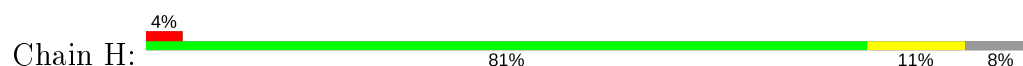
- Molecule 1: Acetylcholine-binding protein



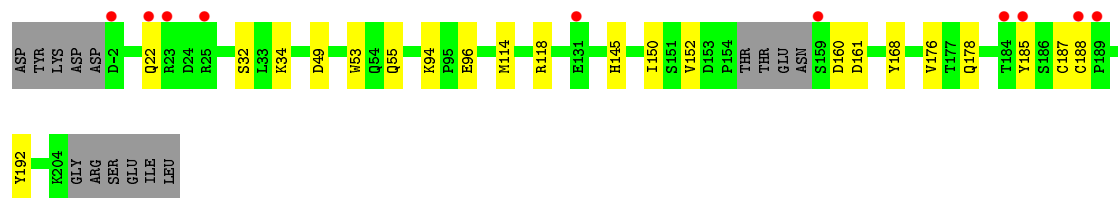
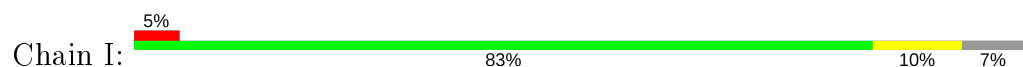
- Molecule 1: Acetylcholine-binding protein



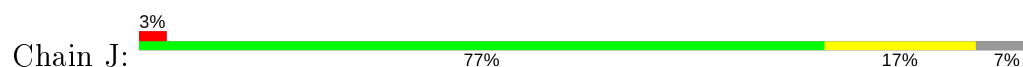
- Molecule 1: Acetylcholine-binding protein

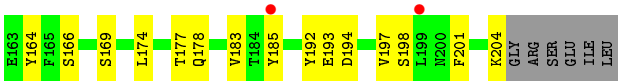


- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.47Å 129.04Å 122.43Å 90.00° 106.28° 90.00°	Depositor
Resolution (Å)	55.16 – 2.40 55.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (55.16-2.40) 99.6 (55.16-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.198 , 0.248 0.203 , 0.251	Depositor DCC
$R_{free}$ test set	4793 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAG, FN1

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	0.47	0/1547	0.64	0/2122
1	B	0.50	0/1620	0.64	0/2221
1	C	0.49	0/1612	0.65	0/2217
1	D	0.48	0/1639	0.64	0/2247
1	E	0.61	0/1572	0.69	0/2158
1	F	0.44	0/1447	0.61	0/1990
1	G	0.59	0/1577	0.66	0/2162
1	H	0.44	0/1616	0.63	0/2208
1	I	0.45	0/1604	0.63	1/2199 (0.0%)
1	J	0.45	0/1522	0.60	0/2099
All	All	0.49	0/15756	0.64	1/21623 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	152	VAL	C-N-CA	8.08	141.90	121.70

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	1513	1421	1419	12	0
1	B	1585	1482	1480	9	0
1	C	1576	1428	1424	9	1
1	D	1604	1503	1503	13	0
1	E	1537	1403	1408	21	0
1	F	1415	1293	1290	21	0
1	G	1542	1438	1438	28	0
1	H	1582	1508	1505	20	0
1	I	1569	1452	1456	13	1
1	J	1487	1329	1326	27	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	J	10	0	0	0	0
3	A	13	14	13	0	0
3	B	13	14	13	1	0
3	C	13	14	13	0	0
3	D	13	14	13	6	0
3	E	13	14	13	4	0
3	F	13	14	13	3	0
3	H	13	14	13	0	0
3	J	13	14	13	6	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
5	A	26	0	0	0	0
5	B	46	0	0	0	0
5	C	43	0	0	1	0
5	D	46	0	0	0	0
5	E	28	0	0	0	0
5	F	16	0	0	0	0
5	G	29	0	0	0	0
5	H	32	0	0	0	0
5	I	37	0	0	0	0
5	J	26	0	0	3	0
All	All	15921	14369	14379	152	1

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 5.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:TYR:OH	5:J:401:HOH:O	2.03	0.76
1:B:3:ARG:NH1	2:B:301:PO4:O2	2.21	0.74
1:J:46:ASN:OD1	1:J:125:VAL:HG22	1.89	0.72
1:E:152:VAL:HG12	1:E:195:VAL:HG23	1.73	0.71
1:F:41:VAL:HG13	1:F:125:VAL:HG21	1.71	0.71
1:I:161:ASP:OD2	1:I:178:GLN:NE2	2.23	0.70
1:G:24:ASP:O	1:H:-2:ASP:OD2	2.13	0.67
1:G:139:LYS:NZ	1:G:185:TYR:OH	2.27	0.67
1:E:152:VAL:CG1	1:E:195:VAL:HG23	2.27	0.65
1:D:192:TYR:CZ	3:D:302:FN1:H102	2.32	0.64
1:F:114:MET:HE2	3:J:303:FN1:H71	1.79	0.64
1:J:183:VAL:HG23	1:J:194:ASP:OD1	1.99	0.63
1:F:94:LYS:HE2	1:G:96:GLU:HG3	1.80	0.62
1:H:41:VAL:HG13	1:H:125:VAL:HG21	1.82	0.62
1:G:152:VAL:CG1	1:G:195:VAL:HG23	2.29	0.62
1:J:183:VAL:HG12	1:J:185:TYR:CE1	2.34	0.62
1:I:32:SER:HA	1:I:178:GLN:HE22	1.65	0.61
1:A:131:GLU:O	1:A:202:ARG:NH1	2.35	0.60
1:J:174:LEU:HD13	1:J:201:PHE:HA	1.84	0.60
1:J:169:SER:O	1:J:204:LYS:NZ	2.33	0.58
1:J:143:TRP:CH2	3:J:303:FN1:H82	2.38	0.58
1:F:124:ASP:HB2	1:G:168:TYR:CE1	2.40	0.57
1:H:41:VAL:CG1	1:H:125:VAL:HG21	2.34	0.57
1:G:152:VAL:HG12	1:G:195:VAL:HG23	1.86	0.56
1:F:30:SER:OG	1:F:57:THR:OG1	2.24	0.56
1:H:42:ASN:HB3	1:H:45:THR:HG22	1.88	0.56
1:A:118:ARG:NH1	1:E:92:ILE:O	2.37	0.55
1:B:19:ILE:HG13	1:B:21:THR:HG23	1.88	0.55
1:J:48:VAL:HG12	1:J:50:VAL:HG13	1.89	0.55
1:A:170:ARG:NH1	1:E:44:ILE:CG2	2.70	0.54
1:H:125:VAL:HA	1:H:134:ALA:HB1	1.90	0.54
1:I:34:LYS:HB2	1:I:53:TRP:HB2	1.90	0.54
1:E:187:CYS:SG	1:E:188:CYS:N	2.81	0.54
1:C:186:SER:OG	1:D:160:ASP:OD2	2.16	0.53
1:F:173:ILE:HD12	1:F:199:LEU:HD11	1.89	0.53
1:G:42:ASN:CG	1:G:45:THR:HG22	2.28	0.53
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.90	0.53
1:C:101:GLN:OE1	1:C:113:TYR:OH	2.25	0.53
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.45	0.52
1:F:94:LYS:HE2	1:G:96:GLU:CG	2.40	0.52
1:J:166:SER:OG	5:J:402:HOH:O	2.18	0.51
1:J:33:LEU:HD11	1:J:140:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:O	1:A:128:VAL:HG23	2.09	0.51
1:D:187:CYS:SG	1:D:188:CYS:N	2.83	0.51
1:E:143:TRP:CZ3	3:E:301:FN1:H82	2.45	0.51
1:E:48:VAL:HG12	1:E:50:VAL:HG13	1.91	0.51
1:J:178:GLN:HG2	1:J:197:VAL:HG22	1.91	0.51
3:D:302:FN1:H71	1:E:114:MET:CE	2.41	0.51
1:C:152:VAL:CG1	1:C:195:VAL:HG23	2.41	0.51
1:A:186:SER:OG	1:B:157:GLU:OE2	2.29	0.50
1:C:48:VAL:HG12	1:C:50:VAL:HG13	1.93	0.50
1:F:145:HIS:HB2	1:F:150:ILE:HD12	1.92	0.50
1:F:34:LYS:HB3	1:F:164:TYR:CD2	2.47	0.50
1:B:152:VAL:HG12	1:B:195:VAL:HG23	1.93	0.49
1:E:188:CYS:SG	3:E:301:FN1:H3	2.52	0.49
1:E:125:VAL:O	1:E:128:VAL:HG23	2.11	0.49
1:F:41:VAL:CG1	1:F:125:VAL:HG21	2.40	0.49
1:G:125:VAL:HG12	1:G:125:VAL:O	2.12	0.48
1:D:143:TRP:CZ3	3:D:302:FN1:H82	2.49	0.48
1:G:55:GLN:HG3	1:G:114:MET:HE3	1.95	0.48
1:F:24:ASP:HA	1:G:-2:ASP:HB2	1.95	0.48
1:H:94:LYS:HE3	1:I:96:GLU:HG3	1.96	0.47
1:J:130:THR:HG22	1:J:132:SER:H	1.79	0.47
3:F:301:FN1:C7	1:G:114:MET:SD	3.02	0.47
1:F:43:GLU:HA	1:F:125:VAL:CG1	2.45	0.47
1:E:55:GLN:HA	1:E:114:MET:HG3	1.96	0.47
1:G:20:PRO:HA	1:H:0:LYS:HD2	1.95	0.47
1:B:33:LEU:HD21	1:B:140:ILE:HD12	1.96	0.47
1:D:158:ASN:HD21	1:D:178:GLN:HB2	1.80	0.47
1:E:192:TYR:CE1	3:E:301:FN1:H103	2.50	0.47
1:H:57:THR:CG2	1:H:112:LEU:HD12	2.45	0.47
1:I:192:TYR:N	1:I:192:TYR:CD1	2.83	0.47
1:C:145:HIS:HB2	1:C:150:ILE:HD12	1.96	0.47
1:D:192:TYR:CE1	3:D:302:FN1:C10	2.98	0.46
3:F:301:FN1:H71	1:G:114:MET:SD	2.56	0.46
1:G:89:TYR:HB2	1:G:139:LYS:HG3	1.97	0.46
1:J:192:TYR:CE2	3:J:303:FN1:H102	2.51	0.46
1:D:152:VAL:HG23	1:D:195:VAL:HG23	1.98	0.46
1:G:41:VAL:HG22	1:G:48:VAL:HG23	1.97	0.46
1:J:192:TYR:CZ	3:J:303:FN1:H102	2.51	0.46
1:C:70:SER:HB2	1:C:71:PRO:HD2	1.96	0.46
1:G:143:TRP:CE2	1:H:99:THR:HG21	2.51	0.46
1:H:-3:ASP:O	1:H:3:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:SER:OG	1:E:37:ASN:ND2	2.49	0.46
1:J:174:LEU:HD12	1:J:174:LEU:N	2.30	0.46
1:A:170:ARG:HH11	1:E:44:ILE:HG22	1.80	0.46
1:F:17:ASP:OD2	1:G:11:ARG:NH2	2.43	0.45
1:H:121:PHE:CD1	1:H:138:ILE:HD12	2.51	0.45
1:C:152:VAL:HG12	1:C:195:VAL:HG23	1.98	0.45
1:E:152:VAL:HG12	1:E:195:VAL:CG2	2.43	0.45
1:J:152:VAL:HG21	1:J:194:ASP:HA	1.99	0.45
1:J:101:GLN:NE2	5:J:401:HOH:O	2.21	0.45
1:F:181:ASN:OD1	1:F:182:SER:N	2.49	0.45
1:I:94:LYS:HE3	1:J:96:GLU:HG2	1.98	0.44
1:I:49:ASP:OD2	1:I:118:ARG:NH2	2.49	0.44
1:F:131:GLU:O	1:F:202:ARG:NH1	2.50	0.44
1:H:125:VAL:O	1:H:125:VAL:HG22	2.17	0.44
1:D:183:VAL:HG11	1:D:185:TYR:CZ	2.53	0.44
1:E:70:SER:HB2	1:E:71:PRO:HD2	1.99	0.44
1:F:165:PHE:CE1	1:F:173:ILE:HD11	2.53	0.44
1:G:70:SER:HB2	1:G:71:PRO:HD2	2.00	0.44
1:J:143:TRP:CZ3	3:J:303:FN1:H82	2.53	0.44
1:D:88:ALA:HA	1:D:139:LYS:O	2.17	0.44
1:F:114:MET:HE2	3:J:303:FN1:C7	2.47	0.44
1:I:55:GLN:HA	1:I:114:MET:HG3	2.00	0.44
1:A:114:MET:CE	3:E:301:FN1:H72	2.49	0.43
1:G:13:THR:HG21	1:G:62:THR:O	2.18	0.43
1:H:51:VAL:HA	1:H:117:ILE:O	2.18	0.43
1:G:173:ILE:HG21	1:G:176:VAL:HG23	2.00	0.43
1:G:42:ASN:HB3	1:G:45:THR:HG22	1.99	0.43
1:H:43:GLU:HA	1:H:125:VAL:HG13	2.00	0.43
1:C:17:ASP:OD2	1:D:11:ARG:NH2	2.37	0.43
1:H:124:ASP:HB2	1:I:168:TYR:CE1	2.53	0.43
1:J:152:VAL:HG22	1:J:193:GLU:CB	2.48	0.43
1:J:99:THR:HG23	1:J:116:SER:HB3	2.00	0.43
1:I:185:TYR:HD2	1:J:164:TYR:HE1	1.67	0.42
1:F:70:SER:HB2	1:F:71:PRO:HD2	2.01	0.42
1:G:167:GLN:O	1:G:204:LYS:NZ	2.52	0.42
1:B:185:TYR:C	1:B:187:CYS:N	2.73	0.42
1:E:176:VAL:HA	1:E:198:SER:O	2.20	0.42
1:I:145:HIS:HB3	1:I:150:ILE:HG13	2.01	0.42
3:D:302:FN1:C7	1:E:114:MET:CE	2.98	0.42
1:J:43:GLU:HA	1:J:125:VAL:HG21	2.02	0.42
1:E:172:GLU:OE1	1:E:202:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TRP:CE2	1:B:99:THR:HG21	2.55	0.41
1:F:38:ILE:HD12	1:F:165:PHE:CZ	2.55	0.41
1:H:57:THR:HG22	1:H:112:LEU:HD12	2.02	0.41
1:F:133:GLY:HA2	1:F:202:ARG:HB3	2.03	0.41
1:G:139:LYS:HA	1:G:195:VAL:O	2.20	0.41
1:I:161:ASP:HB2	1:I:176:VAL:HG11	2.02	0.41
1:E:135:THR:HG22	1:E:200:ASN:HB2	2.03	0.41
1:A:55:GLN:HA	1:A:114:MET:HG3	2.02	0.41
1:G:165:PHE:CD1	1:G:173:ILE:HD11	2.56	0.41
1:I:32:SER:CA	1:I:178:GLN:HE22	2.33	0.41
3:F:301:FN1:H72	1:G:114:MET:SD	2.60	0.41
1:J:65:TRP:CZ3	1:J:107:SER:HA	2.55	0.41
1:F:164:TYR:HE1	1:J:185:TYR:HD2	1.67	0.41
1:G:192:TYR:N	1:G:192:TYR:CD1	2.89	0.41
1:E:9:ASN:O	1:E:13:THR:HG22	2.21	0.41
1:G:33:LEU:H	1:G:178:GLN:HE22	1.67	0.41
1:J:48:VAL:O	1:J:120:ARG:HA	2.21	0.41
1:A:34:LYS:HB3	1:A:164:TYR:CD2	2.56	0.41
3:B:303:FN1:H5	5:C:430:HOH:O	2.20	0.41
1:D:42:ASN:OD1	1:D:44:ILE:HB	2.20	0.41
1:H:183:VAL:HG12	1:H:184:THR:N	2.35	0.41
1:H:42:ASN:CG	1:H:45:THR:HG22	2.42	0.41
1:A:85:ASP:OD1	1:A:85:ASP:N	2.52	0.40
1:H:42:ASN:CB	1:H:45:THR:HG22	2.50	0.40
1:J:177:THR:OG1	1:J:198:SER:HB2	2.21	0.40
1:C:110:GLU:OE1	1:C:112:LEU:HD21	2.22	0.40
1:D:192:TYR:CZ	3:D:302:FN1:C10	3.02	0.40
1:H:88:ALA:HA	1:H:139:LYS:O	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	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:HIS:HE2	1:I:160:ASP:OD2[1_455]	1.54	0.06

## 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	195/218 (89%)	194 (100%)	1 (0%)	0	100	100
1	B	201/218 (92%)	199 (99%)	2 (1%)	0	100	100
1	C	204/218 (94%)	202 (99%)	2 (1%)	0	100	100
1	D	205/218 (94%)	201 (98%)	4 (2%)	0	100	100
1	E	198/218 (91%)	195 (98%)	3 (2%)	0	100	100
1	F	187/218 (86%)	183 (98%)	4 (2%)	0	100	100
1	G	197/218 (90%)	192 (98%)	5 (2%)	0	100	100
1	H	197/218 (90%)	193 (98%)	4 (2%)	0	100	100
1	I	199/218 (91%)	194 (98%)	5 (2%)	0	100	100
1	J	199/218 (91%)	197 (99%)	2 (1%)	0	100	100
All	All	1982/2180 (91%)	1950 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	168/204 (82%)	168 (100%)	0	100	100
1	B	181/204 (89%)	180 (99%)	1 (1%)	86	94
1	C	175/204 (86%)	174 (99%)	1 (1%)	86	94
1	D	183/204 (90%)	181 (99%)	2 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	170/204 (83%)	169 (99%)	1 (1%)	86	94
1	F	148/204 (72%)	147 (99%)	1 (1%)	84	92
1	G	173/204 (85%)	171 (99%)	2 (1%)	71	85
1	H	180/204 (88%)	179 (99%)	1 (1%)	86	94
1	I	178/204 (87%)	175 (98%)	3 (2%)	60	78
1	J	158/204 (78%)	156 (99%)	2 (1%)	69	84
All	All	1714/2040 (84%)	1700 (99%)	14 (1%)	81	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	C	182	SER
1	D	83	VAL
1	D	126	SER
1	E	187	CYS
1	F	99	THR
1	G	21	THR
1	G	153	ASP
1	H	83	VAL
1	I	22	GLN
1	I	187	CYS
1	I	188	CYS
1	J	56	THR
1	J	151	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	158	ASN
1	E	146	HIS
1	G	9	ASN
1	H	69	HIS
1	H	200	ASN
1	I	178	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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$
3	FN1	D	302	-	14,14,14	3.94	6 (42%)	19,19,19	1.88	6 (31%)
2	PO4	D	301	-	4,4,4	1.18	0	6,6,6	0.53	0
2	PO4	A	301	-	4,4,4	0.89	0	6,6,6	0.70	0
2	PO4	B	301	-	4,4,4	0.89	0	6,6,6	0.63	0
2	PO4	G	301	-	4,4,4	0.95	0	6,6,6	0.79	0
2	PO4	H	301	-	4,4,4	0.91	0	6,6,6	0.38	0
3	FN1	F	301	-	14,14,14	3.76	7 (50%)	19,19,19	1.87	8 (42%)
3	FN1	C	302	-	14,14,14	3.82	7 (50%)	19,19,19	1.72	7 (36%)
3	FN1	B	303	-	14,14,14	3.90	7 (50%)	19,19,19	1.87	6 (31%)
2	PO4	B	302	-	4,4,4	1.16	0	6,6,6	0.60	0
4	NAG	A	303	1	14,14,15	0.69	0	17,19,21	1.41	3 (17%)
2	PO4	J	302	-	4,4,4	0.93	0	6,6,6	0.57	0
3	FN1	H	303	-	14,14,14	3.84	7 (50%)	19,19,19	1.84	4 (21%)
4	NAG	C	303	1	14,14,15	1.36	1 (7%)	17,19,21	0.99	0
3	FN1	J	303	-	14,14,14	3.97	7 (50%)	19,19,19	1.80	7 (36%)
2	PO4	C	301	-	4,4,4	0.98	0	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	J	301	-	4,4,4	0.82	0	6,6,6	0.79	0
3	FN1	E	301	-	14,14,14	3.75	7 (50%)	19,19,19	1.71	6 (31%)
2	PO4	H	302	-	4,4,4	0.89	0	6,6,6	0.89	0
3	FN1	A	302	-	14,14,14	3.76	7 (50%)	19,19,19	1.86	6 (31%)

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	FN1	D	302	-	-	3/4/14/14	0/2/2/2
3	FN1	C	302	-	-	4/4/14/14	0/2/2/2
4	NAG	A	303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	303	1	-	0/6/23/26	0/1/1/1
3	FN1	B	303	-	-	0/4/14/14	0/2/2/2
3	FN1	E	301	-	-	2/4/14/14	0/2/2/2
3	FN1	H	303	-	-	0/4/14/14	0/2/2/2
3	FN1	J	303	-	-	4/4/14/14	0/2/2/2
3	FN1	F	301	-	-	0/4/14/14	0/2/2/2
3	FN1	A	302	-	-	0/4/14/14	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	303	FN1	C5-C4	9.82	1.51	1.37
3	B	303	FN1	C5-C4	9.30	1.50	1.37
3	A	302	FN1	C5-C4	9.16	1.50	1.37
3	H	303	FN1	C5-C4	9.13	1.50	1.37
3	E	301	FN1	C5-C4	9.10	1.50	1.37
3	D	302	FN1	C5-C4	9.03	1.50	1.37
3	C	302	FN1	C5-C4	8.85	1.50	1.37
3	F	301	FN1	C5-C4	8.67	1.49	1.37
3	D	302	FN1	C3-C2	7.48	1.50	1.39
3	C	302	FN1	C3-C2	7.17	1.50	1.39
3	J	303	FN1	C3-C2	7.09	1.50	1.39
3	E	301	FN1	C3-C2	6.87	1.49	1.39
3	H	303	FN1	C3-C2	6.87	1.49	1.39
3	B	303	FN1	C3-C2	6.66	1.49	1.39
3	F	301	FN1	C3-C2	6.61	1.49	1.39
3	B	303	FN1	C1-N1	6.11	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	FN1	C1-N1	5.94	1.47	1.34
3	D	302	FN1	C1-N1	5.76	1.46	1.34
3	J	303	FN1	C1-N1	5.74	1.46	1.34
3	F	301	FN1	C1-N1	5.73	1.46	1.34
3	H	303	FN1	C1-N1	5.69	1.46	1.34
3	A	302	FN1	C3-C2	5.65	1.48	1.39
3	C	302	FN1	C1-N1	5.45	1.46	1.34
3	E	301	FN1	C1-N1	5.36	1.45	1.34
4	C	303	NAG	O5-C1	4.31	1.50	1.43
3	D	302	FN1	C10-N2	-3.72	1.39	1.46
3	B	303	FN1	C7-C6	-3.57	1.44	1.54
3	C	302	FN1	C7-C6	-3.50	1.45	1.54
3	F	301	FN1	C7-C6	-3.50	1.45	1.54
3	F	301	FN1	C3-C4	-3.43	1.32	1.37
3	J	303	FN1	C7-C6	-3.43	1.45	1.54
3	A	302	FN1	C3-C4	-3.42	1.32	1.37
3	A	302	FN1	C7-C6	-3.37	1.45	1.54
3	D	302	FN1	C7-C6	-3.37	1.45	1.54
3	E	301	FN1	C3-C4	-3.29	1.32	1.37
3	H	303	FN1	C7-C6	-3.26	1.45	1.54
3	J	303	FN1	C3-C4	-3.12	1.32	1.37
3	C	302	FN1	C3-C4	-3.04	1.32	1.37
3	H	303	FN1	C3-C4	-3.03	1.32	1.37
3	B	303	FN1	C3-C4	-3.00	1.32	1.37
3	H	303	FN1	C2-C6	-2.99	1.47	1.51
3	A	302	FN1	C2-C6	-2.98	1.47	1.51
3	E	301	FN1	C7-C6	-2.87	1.46	1.54
3	B	303	FN1	C2-C6	-2.87	1.47	1.51
3	D	302	FN1	C3-C4	-2.86	1.33	1.37
3	C	302	FN1	C2-C6	-2.83	1.47	1.51
3	J	303	FN1	C10-N2	-2.51	1.41	1.46
3	F	301	FN1	C2-C6	-2.46	1.48	1.51
3	B	303	FN1	C10-N2	-2.45	1.41	1.46
3	F	301	FN1	C10-N2	-2.36	1.41	1.46
3	C	302	FN1	C10-N2	-2.33	1.42	1.46
3	E	301	FN1	C2-C6	-2.30	1.48	1.51
3	H	303	FN1	C10-N2	-2.29	1.42	1.46
3	A	302	FN1	C10-N2	-2.28	1.42	1.46
3	E	301	FN1	C10-N2	-2.20	1.42	1.46
3	J	303	FN1	C2-C6	-2.15	1.48	1.51

All (53) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	FN1	C7-C6-C2	-3.89	106.08	113.61
3	A	302	FN1	C7-C6-C2	-3.88	106.10	113.61
3	B	303	FN1	C7-C6-C2	-3.84	106.17	113.61
3	D	302	FN1	C9-N2-C6	3.83	115.97	104.37
3	H	303	FN1	C7-C6-C2	-3.75	106.34	113.61
3	H	303	FN1	C3-C2-C1	3.32	119.66	117.44
3	J	303	FN1	C3-C2-C6	-3.20	114.28	120.42
3	E	301	FN1	C9-N2-C6	3.18	113.98	104.37
3	B	303	FN1	C9-N2-C6	3.10	113.76	104.37
3	F	301	FN1	C9-N2-C6	3.06	113.64	104.37
3	J	303	FN1	C3-C2-C1	3.04	119.47	117.44
3	D	302	FN1	C10-N2-C9	-3.04	103.18	112.70
3	A	302	FN1	C9-N2-C6	3.00	113.46	104.37
3	D	302	FN1	C10-N2-C6	-2.96	103.84	112.83
4	A	303	NAG	O5-C1-C2	-2.92	106.68	111.29
3	C	302	FN1	C9-N2-C6	2.90	113.14	104.37
3	E	301	FN1	C10-N2-C9	-2.81	103.91	112.70
3	H	303	FN1	C9-N2-C6	2.79	112.81	104.37
3	A	302	FN1	C3-C2-C6	-2.69	115.27	120.42
3	J	303	FN1	C9-N2-C6	2.60	112.25	104.37
3	J	303	FN1	C10-N2-C9	-2.48	104.92	112.70
3	F	301	FN1	C10-N2-C9	-2.48	104.94	112.70
3	C	302	FN1	C2-C1-N1	-2.47	120.26	124.14
3	H	303	FN1	C2-C1-N1	-2.46	120.28	124.14
3	D	302	FN1	C2-C3-C4	2.44	121.27	118.80
3	C	302	FN1	C5-N1-C1	2.39	120.75	117.48
3	E	301	FN1	C10-N2-C6	-2.39	105.58	112.83
3	B	303	FN1	C2-C1-N1	-2.38	120.40	124.14
3	E	301	FN1	C3-C2-C6	-2.36	115.89	120.42
3	A	302	FN1	C3-C2-C1	2.30	118.98	117.44
3	J	303	FN1	C1-C2-C6	2.30	126.24	121.40
4	A	303	NAG	O3-C3-C2	2.25	114.11	109.47
3	D	302	FN1	C8-C7-C6	2.25	110.12	104.26
3	J	303	FN1	C8-C9-N2	-2.24	97.56	103.85
3	D	302	FN1	C5-N1-C1	2.23	120.52	117.48
3	A	302	FN1	C10-N2-C9	-2.22	105.74	112.70
3	B	303	FN1	C3-C2-C1	2.22	118.92	117.44
3	F	301	FN1	C2-C1-N1	-2.22	120.66	124.14
3	F	301	FN1	C3-C2-C6	-2.20	116.20	120.42
3	F	301	FN1	C5-N1-C1	2.16	120.43	117.48
3	J	303	FN1	C2-C1-N1	-2.15	120.76	124.14
3	B	303	FN1	C5-N1-C1	2.13	120.39	117.48
4	A	303	NAG	O3-C3-C4	-2.13	105.43	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	FN1	C10-N2-C6	-2.13	106.37	112.83
3	C	302	FN1	C2-C6-N2	-2.12	106.92	112.37
3	C	302	FN1	C2-C3-C4	2.07	120.89	118.80
3	A	302	FN1	C1-C2-C6	2.06	125.75	121.40
3	E	301	FN1	C1-C2-C6	2.05	125.72	121.40
3	B	303	FN1	C10-N2-C9	-2.04	106.30	112.70
3	C	302	FN1	C3-C2-C1	2.02	118.79	117.44
3	E	301	FN1	C2-C6-N2	-2.01	107.20	112.37
3	F	301	FN1	C2-C3-C4	2.01	120.83	118.80
3	F	301	FN1	C8-C7-C6	2.00	109.48	104.26

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	303	FN1	C1-C2-C6-C7
3	J	303	FN1	C1-C2-C6-N2
3	E	301	FN1	C1-C2-C6-C7
4	A	303	NAG	O5-C5-C6-O6
3	E	301	FN1	C3-C2-C6-C7
4	A	303	NAG	C4-C5-C6-O6
3	D	302	FN1	C1-C2-C6-C7
3	C	302	FN1	C1-C2-C6-C7
3	J	303	FN1	C3-C2-C6-N2
3	J	303	FN1	C3-C2-C6-C7
3	D	302	FN1	C3-C2-C6-C7
3	C	302	FN1	C1-C2-C6-N2
3	C	302	FN1	C3-C2-C6-C7
3	C	302	FN1	C3-C2-C6-N2
3	D	302	FN1	C3-C2-C6-N2

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	FN1	6	0
2	B	301	PO4	1	0
3	F	301	FN1	3	0
3	B	303	FN1	1	0
3	J	303	FN1	6	0
3	E	301	FN1	4	0

## 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	199/218 (91%)	0.26	2 (1%) 82 80	33, 46, 63, 72	0
1	B	205/218 (94%)	0.23	3 (1%) 73 72	29, 40, 57, 98	0
1	C	208/218 (95%)	0.20	0 100 100	28, 41, 62, 84	0
1	D	207/218 (94%)	0.25	3 (1%) 75 73	29, 43, 69, 95	0
1	E	202/218 (92%)	0.26	5 (2%) 57 55	28, 48, 77, 89	0
1	F	193/218 (88%)	0.29	8 (4%) 37 36	36, 51, 72, 85	0
1	G	201/218 (92%)	0.44	7 (3%) 44 43	28, 51, 80, 91	0
1	H	201/218 (92%)	0.37	8 (3%) 38 37	36, 52, 77, 93	0
1	I	203/218 (93%)	0.35	10 (4%) 29 28	33, 46, 73, 101	0
1	J	203/218 (93%)	0.38	7 (3%) 45 44	34, 52, 78, 106	0
All	All	2022/2180 (92%)	0.30	53 (2%) 56 54	28, 47, 74, 106	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	183	VAL	5.1
1	J	185	TYR	4.8
1	H	-2	ASP	4.2
1	I	23	ARG	4.1
1	I	184	THR	4.0
1	B	187	CYS	3.7
1	E	188	CYS	3.7
1	G	174	LEU	3.6
1	H	-3	ASP	3.6
1	E	189	PRO	3.5
1	G	164	TYR	3.4
1	D	68	SER	3.2
1	I	159	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	-2	ASP	3.1
1	I	188	CYS	3.0
1	G	190	GLU	2.9
1	H	69	HIS	2.9
1	G	189	PRO	2.9
1	I	22	GLN	2.8
1	H	68	SER	2.8
1	J	199	LEU	2.8
1	D	183	VAL	2.7
1	A	44	ILE	2.7
1	I	185	TYR	2.7
1	H	61	ARG	2.6
1	B	68	SER	2.6
1	E	187	CYS	2.5
1	G	188	CYS	2.5
1	F	184	THR	2.5
1	F	138	ILE	2.5
1	I	189	PRO	2.5
1	J	129	ASP	2.5
1	G	183	VAL	2.4
1	I	25	ARG	2.4
1	B	188	CYS	2.4
1	J	162	SER	2.3
1	J	132	SER	2.3
1	D	48	VAL	2.2
1	J	44	ILE	2.2
1	F	174	LEU	2.2
1	F	133	GLY	2.2
1	A	154	PRO	2.1
1	H	23	ARG	2.1
1	F	132	SER	2.1
1	E	128	VAL	2.1
1	E	199	LEU	2.1
1	G	48	VAL	2.0
1	F	153	ASP	2.0
1	H	162	SER	2.0
1	H	25	ARG	2.0
1	F	162	SER	2.0
1	J	68	SER	2.0
1	I	131	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FN1	J	303	13/13	0.79	0.28	56,70,82,86	0
3	FN1	F	301	13/13	0.80	0.35	53,64,76,79	0
3	FN1	B	303	13/13	0.84	0.25	46,57,68,71	0
4	NAG	A	303	14/15	0.85	0.23	42,53,57,58	0
3	FN1	D	302	13/13	0.86	0.22	48,65,81,81	0
3	FN1	E	301	13/13	0.87	0.28	51,65,80,80	0
4	NAG	C	303	14/15	0.91	0.26	38,42,48,48	0
3	FN1	A	302	13/13	0.91	0.16	37,52,63,71	0
3	FN1	H	303	13/13	0.94	0.16	44,57,69,69	0
3	FN1	C	302	13/13	0.96	0.21	40,50,61,61	0
2	PO4	H	301	5/5	0.97	0.15	35,38,48,51	0
2	PO4	B	301	5/5	0.98	0.17	41,43,46,49	0
2	PO4	A	301	5/5	0.98	0.15	36,37,42,47	0
2	PO4	J	301	5/5	0.98	0.18	35,41,43,46	0
2	PO4	C	301	5/5	0.99	0.15	36,36,37,37	0
2	PO4	G	301	5/5	0.99	0.15	37,39,44,48	0
2	PO4	H	302	5/5	0.99	0.15	36,39,42,42	0
2	PO4	B	302	5/5	0.99	0.18	28,30,33,35	0
2	PO4	J	302	5/5	0.99	0.15	36,38,45,46	0
2	PO4	D	301	5/5	1.00	0.18	34,35,45,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.