



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:54 PM GMT

PDB ID : 4ZJT  
Title : X-ray crystal structure of Lymnaea stagnalis acetylcholine binding protein (LsAChBP) in complex with 2-Thiophenylmethylene Anabaseine (2TAB)  
Authors : Bobango, J.; Wu, J.; Talley, T.T.  
Deposited on : 2015-04-29  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

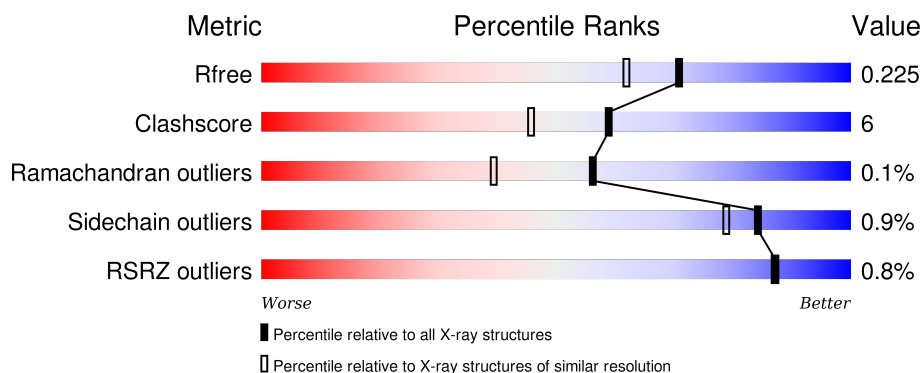
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	B	218	<div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	C	218	<div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	D	218	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	E	218	<div> <div>87%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	<div><div></div><div>86%</div><div>12%</div><div></div><div>•</div></div>
1	G	218	<div><div></div><div>89%</div><div>8%</div><div></div><div>••</div></div>
1	H	218	<div><div>2%</div><div></div><div>84%</div><div>11%</div><div>5%</div><div></div></div>
1	I	218	<div><div></div><div>82%</div><div>15%</div><div></div><div>•</div></div>
1	J	218	<div><div>2%</div><div></div><div>87%</div><div>10%</div><div></div><div>•</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17593 atoms, of which 140 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	212	Total	C	N	O	S	0	1	0
			1674	1048	282	339	5			
1	B	210	Total	C	N	O	S	0	1	0
			1655	1034	279	337	5			
1	C	209	Total	C	N	O	S	0	1	0
			1645	1032	276	332	5			
1	D	214	Total	C	N	O	S	0	0	0
			1674	1046	278	345	5			
1	E	212	Total	C	N	O	S	0	0	0
			1641	1028	275	333	5			
1	F	214	Total	C	N	O	S	0	0	0
			1660	1039	278	338	5			
1	G	214	Total	C	N	O	S	0	1	0
			1670	1045	278	342	5			
1	H	208	Total	C	N	O	S	0	1	0
			1651	1032	283	331	5			
1	I	211	Total	C	N	O	S	0	0	0
			1637	1025	270	337	5			
1	J	211	Total	C	N	O	S	0	0	0
			1660	1036	277	342	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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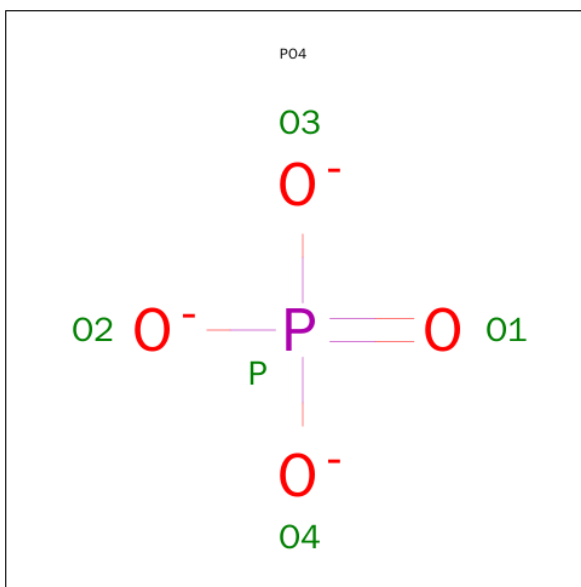
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP P58154
B	-5	LYS	-	expression tag	UNP P58154
B	-4	ASP	-	expression tag	UNP P58154
B	-3	ASP	-	expression tag	UNP P58154
B	-2	ASP	-	expression tag	UNP P58154
B	-1	ASP	-	expression tag	UNP P58154
B	0	LYS	-	expression tag	UNP P58154
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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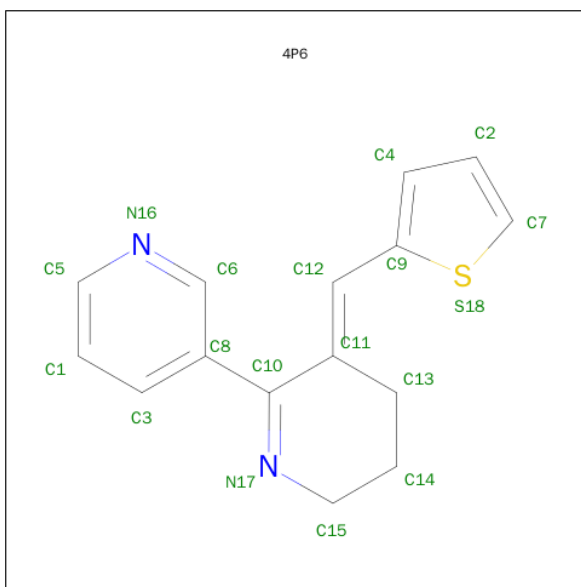
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
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	A	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	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is (3E)-3-(thiophen-2-ylmethylidene)-3,4,5,6-tetrahydro-2,3'-bipyridine (three-letter code: 4P6) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	B	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	C	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	D	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	E	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	F	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	G	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	H	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	I	1	Total	C	H	N	S	0	0
			32	15	14	2	1		
3	J	1	Total	C	H	N	S	0	0
			32	15	14	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	67	Total	O	0	0
			67	67		

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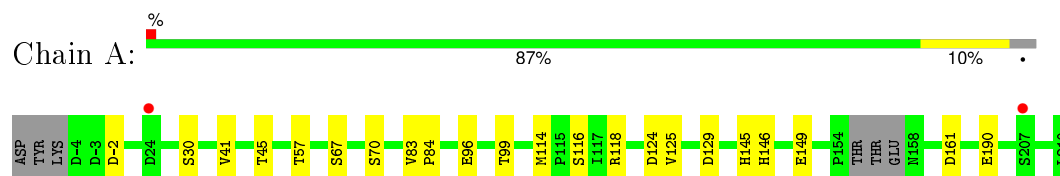
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	64	Total 64	O 64	0	0
4	D	75	Total 75	O 75	0	0
4	E	52	Total 52	O 52	0	0
4	F	67	Total 67	O 67	0	0
4	G	67	Total 67	O 67	0	0
4	H	62	Total 62	O 62	0	0
4	I	70	Total 70	O 70	0	0
4	J	78	Total 78	O 78	0	0

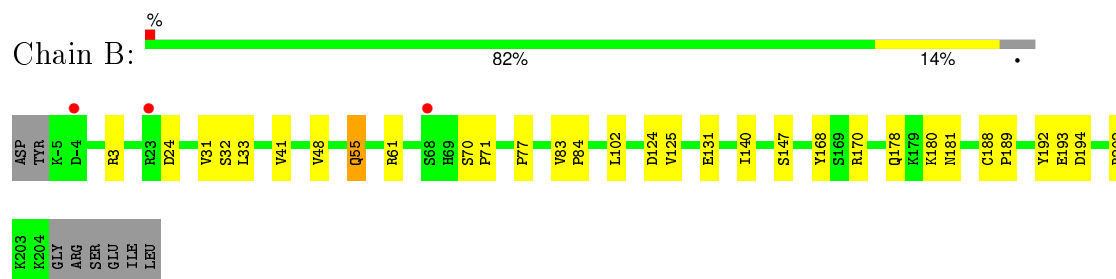
### 3 Residue-property plots

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

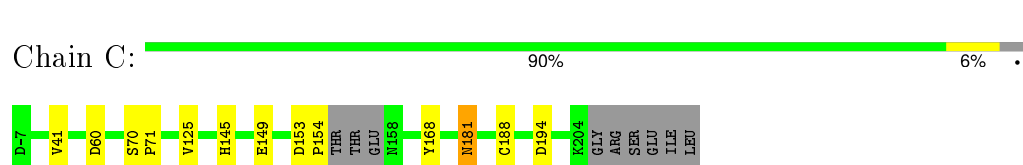
- Molecule 1: Acetylcholine-binding protein



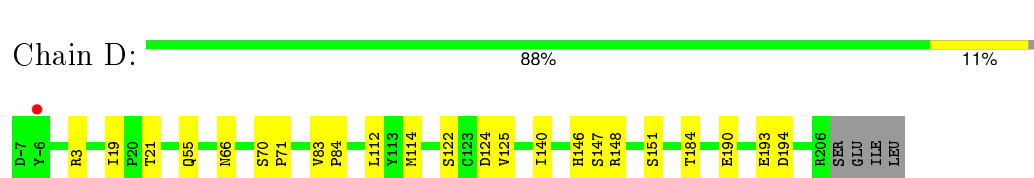
- Molecule 1: Acetylcholine-binding protein



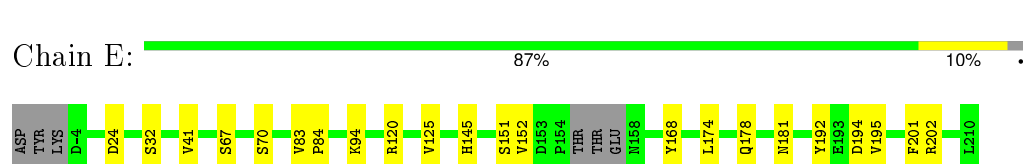
- Molecule 1: Acetylcholine-binding protein



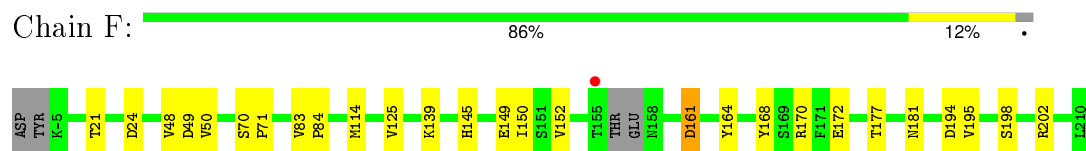
- Molecule 1: Acetylcholine-binding protein



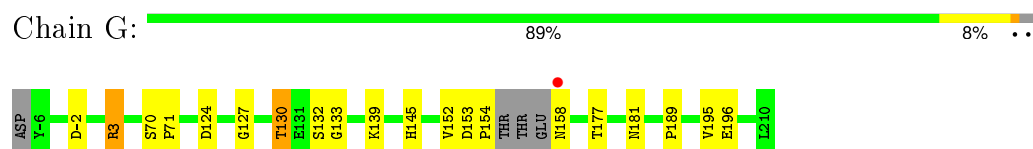
- Molecule 1: Acetylcholine-binding protein



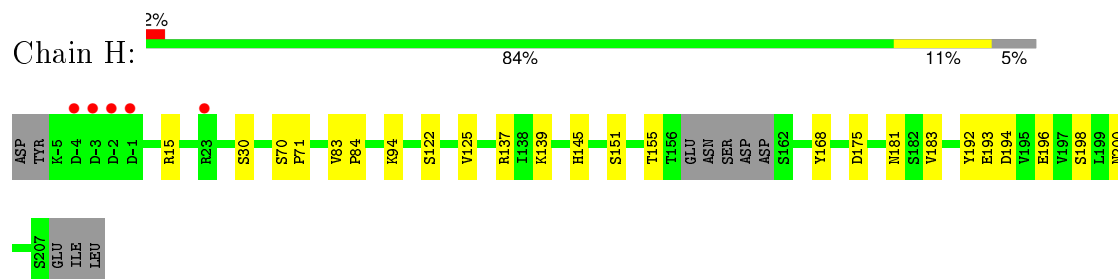
- Molecule 1: Acetylcholine-binding protein



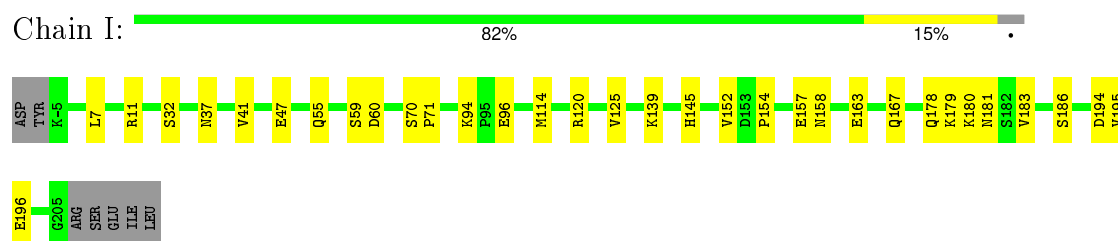
- Molecule 1: Acetylcholine-binding protein



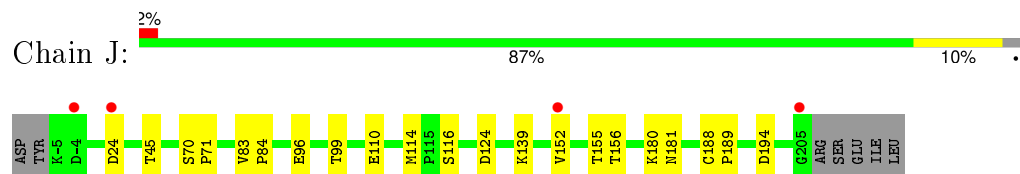
- Molecule 1: Acetylcholine-binding protein



- 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, $\alpha$ , $\beta$ , $\gamma$	85.84Å 127.60Å 122.47Å 90.00° 110.45° 90.00°	Depositor
Resolution (Å)	49.98 – 1.85 49.99 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.98-1.85) 88.9 (49.99-1.74)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.74Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.189 , 0.225 0.197 , 0.225	Depositor DCC
$R_{free}$ test set	1739 reflections (0.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 44.0	EDS
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 241276 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4P6, PO4

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	0.34	0/1713	0.51	0/2339
1	B	0.39	0/1694	0.54	0/2317
1	C	0.36	0/1685	0.51	0/2304
1	D	0.37	0/1711	0.56	0/2342
1	E	0.33	0/1676	0.49	0/2294
1	F	0.35	0/1695	0.51	0/2319
1	G	0.36	0/1708	0.55	1/2335 (0.0%)
1	H	0.38	0/1689	0.54	0/2305
1	I	0.38	0/1673	0.55	0/2291
1	J	0.38	0/1696	0.54	0/2319
All	All	0.36	0/16940	0.53	1/23165 (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	G	3	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1674	0	1590	24	0
1	B	1655	0	1568	24	0
1	C	1645	0	1548	10	0
1	D	1674	0	1564	14	0
1	E	1641	0	1538	19	0
1	F	1660	0	1560	20	0
1	G	1670	0	1570	14	0
1	H	1651	0	1584	19	0
1	I	1637	0	1534	26	0
1	J	1660	0	1568	18	0
2	A	10	0	0	2	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	G	10	0	0	2	0
2	I	10	0	0	2	0
2	J	5	0	0	0	0
3	A	18	14	14	3	0
3	B	18	14	14	4	0
3	C	18	14	14	0	0
3	D	18	14	14	3	0
3	E	18	14	14	6	0
3	F	18	14	14	2	0
3	G	18	14	14	1	0
3	H	18	14	14	1	0
3	I	18	14	14	3	0
3	J	18	14	14	3	0
4	A	54	0	0	0	0
4	B	67	0	0	3	0
4	C	64	0	0	1	0
4	D	75	0	0	1	0
4	E	52	0	0	1	0
4	F	67	0	0	0	0
4	G	67	0	0	0	0
4	H	62	0	0	1	0
4	I	70	0	0	3	0
4	J	78	0	0	1	0
All	All	17453	140	15764	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (188) 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:E:152:VAL:HG12	1:E:195:VAL:HG23	1.59	0.84
1:A:146[B]:HIS:CD2	1:A:190:GLU:HG3	2.13	0.83
1:F:139:LYS:HE2	1:F:181:ASN:ND2	2.01	0.76
1:C:149:GLU:OE2	1:D:3:ARG:NH2	2.19	0.75
1:H:181:ASN:HB3	1:H:194:ASP:OD1	1.88	0.73
1:H:94:LYS:HE3	1:I:96:GLU:HG2	1.70	0.73
1:F:177:THR:HG22	1:F:198:SER:HB2	1.69	0.72
3:E:301:4P6:S18	3:E:301:4P6:H27	2.29	0.72
1:F:177:THR:CG2	1:F:198:SER:HB2	2.20	0.72
1:A:146[B]:HIS:CG	1:A:190:GLU:HG3	2.25	0.71
1:B:180:LYS:NZ	4:B:403:HOH:O	2.24	0.70
1:J:139:LYS:HE2	1:J:181:ASN:ND2	2.07	0.69
1:I:181:ASN:HB3	1:I:194:ASP:OD1	1.92	0.69
1:H:139:LYS:HG2	1:H:196:GLU:OE1	1.93	0.69
1:F:170:ARG:HD2	1:J:45:THR:HA	1.78	0.66
1:H:137:ARG:NH1	1:H:198:SER:OG	2.29	0.65
1:F:181:ASN:HB3	1:F:194:ASP:OD1	1.96	0.65
1:H:183:VAL:HG13	1:H:192:TYR:HB2	1.78	0.65
1:C:60:ASP:OD2	4:C:401:HOH:O	2.15	0.64
1:B:83:VAL:HG13	1:B:84:PRO:HD2	1.80	0.64
1:I:70:SER:HB2	1:I:71:PRO:HD2	1.79	0.64
1:A:149:GLU:OE2	1:B:3:ARG:NH2	2.24	0.64
1:H:70:SER:HB2	1:H:71:PRO:HD2	1.80	0.64
1:G:139:LYS:HE2	1:G:181:ASN:ND2	2.13	0.63
1:I:47:GLU:OE1	1:I:120:ARG:NH2	2.32	0.62
3:D:302:4P6:C13	3:D:302:4P6:S18	2.87	0.62
1:A:83:VAL:HG13	1:A:84:PRO:HD2	1.81	0.62
1:J:152:VAL:HG21	1:J:194:ASP:HA	1.82	0.61
1:G:127:GLY:O	1:G:130:THR:HB	2.01	0.60
1:J:83:VAL:HG13	1:J:84:PRO:HD2	1.83	0.60
1:A:45:THR:HG22	1:B:170:ARG:NH1	2.17	0.60
3:A:303:4P6:C3	3:A:303:4P6:H26	2.31	0.59
3:A:303:4P6:S18	3:A:303:4P6:H28	2.42	0.59
1:I:41:VAL:HG13	1:I:125:VAL:HG11	1.84	0.59
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.37	0.59
1:F:48:VAL:HG12	1:F:50:VAL:HG13	1.83	0.59
1:H:183:VAL:CG1	1:H:192:TYR:HB2	2.32	0.59
1:H:183:VAL:HG12	1:H:192:TYR:O	2.03	0.59
1:D:70:SER:HB2	1:D:71:PRO:HD2	1.84	0.59
3:A:303:4P6:S18	3:A:303:4P6:C13	2.91	0.59
1:F:83:VAL:HG13	1:F:84:PRO:HD2	1.83	0.58
1:E:174:LEU:HD11	1:E:202:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:VAL:HG12	1:I:195:VAL:HG23	1.84	0.58
1:D:66:ASN:ND2	4:D:401:HOH:O	2.32	0.57
1:A:41:VAL:CG1	1:A:125:VAL:HG11	2.35	0.57
3:B:302:4P6:S18	3:B:302:4P6:C13	2.93	0.56
3:J:302:4P6:C13	3:J:302:4P6:S18	2.95	0.55
1:G:70:SER:HB2	1:G:71:PRO:HD2	1.90	0.54
1:I:7:LEU:O	1:I:11:ARG:HG3	2.07	0.54
3:F:301:4P6:S18	3:F:301:4P6:C13	2.96	0.54
1:H:122:SER:HB2	1:I:37:ASN:ND2	2.22	0.54
1:F:21:THR:OG1	1:G:-2:ASP:HB3	2.06	0.54
1:H:94:LYS:HE3	1:I:96:GLU:CG	2.37	0.54
1:F:152:VAL:HG12	1:F:195:VAL:HG23	1.89	0.53
1:C:181:ASN:HB3	1:C:194:ASP:OD2	2.08	0.53
1:A:-2:ASP:HB2	1:E:24:ASP:HA	1.91	0.53
3:D:302:4P6:H28	3:D:302:4P6:S18	2.50	0.52
1:E:32:SER:HA	1:E:178:GLN:HE22	1.74	0.52
3:E:301:4P6:S18	3:E:301:4P6:C13	2.97	0.52
1:A:114:MET:CE	3:E:301:4P6:C12	2.88	0.51
1:A:146[B]:HIS:CE1	1:A:190:GLU:CG	2.94	0.51
3:B:302:4P6:H28	3:B:302:4P6:S18	2.51	0.51
1:D:125:VAL:HG12	1:D:125:VAL:O	2.09	0.51
1:J:110:GLU:OE2	4:J:401:HOH:O	2.19	0.51
1:A:146[B]:HIS:CE1	1:A:190:GLU:HG3	2.46	0.51
1:I:157:GLU:HG2	1:I:158:ASN:N	2.26	0.51
1:I:70:SER:HB2	1:I:71:PRO:CD	2.41	0.50
1:B:181:ASN:HB3	1:B:194:ASP:OD1	2.12	0.50
1:I:60:ASP:OD2	4:I:401:HOH:O	2.19	0.50
1:D:146:HIS:CE1	1:D:148:ARG:HB2	2.46	0.50
1:F:70:SER:HB2	1:F:71:PRO:HD2	1.93	0.50
1:A:146[B]:HIS:NE2	1:A:190:GLU:HG3	2.27	0.50
1:B:83:VAL:CG1	1:B:84:PRO:HD2	2.41	0.50
3:I:303:4P6:C12	1:J:114:MET:CE	2.90	0.50
1:I:154:PRO:HG3	1:I:180:LYS:HB2	1.94	0.50
1:D:83:VAL:HG13	1:D:84:PRO:HD2	1.93	0.50
3:B:302:4P6:H26	3:B:302:4P6:C3	2.40	0.50
1:B:125:VAL:HG12	1:B:125:VAL:O	2.11	0.50
1:H:70:SER:HB2	1:H:71:PRO:CD	2.41	0.50
1:B:170:ARG:NH2	4:B:405:HOH:O	2.43	0.50
1:J:70:SER:HB2	1:J:71:PRO:HD2	1.94	0.49
1:E:174:LEU:HD13	1:E:201:PHE:HA	1.94	0.49
1:B:70:SER:HB2	1:B:71:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ARG:NH1	4:E:402:HOH:O	2.44	0.49
1:D:55:GLN:HG3	1:D:114:MET:SD	2.53	0.49
1:G:130:THR:HG22	1:G:132:SER:H	1.78	0.49
3:F:301:4P6:H26	3:F:301:4P6:C3	2.42	0.48
1:I:94:LYS:HE3	1:J:96:GLU:HG3	1.95	0.48
1:E:174:LEU:HD12	1:E:174:LEU:N	2.28	0.48
3:D:302:4P6:H26	3:D:302:4P6:C3	2.42	0.48
1:J:70:SER:HB2	1:J:71:PRO:CD	2.43	0.48
1:G:158:ASN:OD1	1:G:177:THR:HG22	2.14	0.48
1:H:151:SER:HB2	1:H:193:GLU:OE1	2.13	0.48
1:A:41:VAL:CG1	1:A:125:VAL:CG1	2.91	0.48
1:E:125:VAL:HG12	1:E:125:VAL:O	2.14	0.48
1:A:96:GLU:HG3	1:E:94:LYS:HD2	1.95	0.48
1:J:181:ASN:ND2	1:J:194:ASP:OD1	2.40	0.48
1:I:125:VAL:HG12	1:I:125:VAL:O	2.13	0.47
1:D:70:SER:HB2	1:D:71:PRO:CD	2.44	0.47
1:E:181:ASN:HB3	1:E:194:ASP:OD1	2.13	0.47
1:A:114:MET:HE2	3:E:301:4P6:C12	2.44	0.47
1:A:125:VAL:O	1:A:125:VAL:HG12	2.13	0.47
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.49	0.47
1:A:83:VAL:CG1	1:A:84:PRO:HD2	2.44	0.47
1:B:31:VAL:HA	1:B:55:GLN:O	2.14	0.47
1:H:83:VAL:HG13	1:H:84:PRO:HD2	1.95	0.47
1:H:30:SER:HB3	1:H:155:THR:HG22	1.96	0.47
1:G:139:LYS:HE3	1:G:196:GLU:OE1	2.15	0.47
1:E:192:TYR:OH	3:E:301:4P6:H21	2.14	0.47
3:H:301:4P6:C13	3:H:301:4P6:S18	3.03	0.47
1:I:163:GLU:HG2	4:I:464:HOH:O	2.14	0.46
1:J:152:VAL:CG2	1:J:194:ASP:HA	2.44	0.46
3:I:303:4P6:C13	3:I:303:4P6:S18	3.04	0.46
2:A:301:PO4:O2	1:E:145:HIS:HE1	1.98	0.46
1:J:188:CYS:HB3	1:J:189:PRO:HD2	1.97	0.46
1:B:147:SER:HB3	1:B:193:GLU:HG3	1.97	0.46
3:G:303:4P6:S18	3:G:303:4P6:C13	3.04	0.46
1:I:145:HIS:HE1	2:I:302:PO4:O2	1.99	0.46
3:I:303:4P6:C12	1:J:114:MET:HE2	2.45	0.45
1:F:83:VAL:CG1	1:F:84:PRO:HD2	2.46	0.45
1:B:193:GLU:O	4:B:402:HOH:O	2.20	0.45
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.51	0.45
1:C:125:VAL:HG12	1:C:125:VAL:O	2.16	0.45
1:A:41:VAL:HG12	1:A:125:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:SER:HA	1:E:70:SER:OG	2.17	0.44
1:A:30:SER:HB2	1:A:57:THR:OG1	2.17	0.44
1:D:140:ILE:O	1:D:194:ASP:HB2	2.17	0.44
1:A:145:HIS:HE1	2:A:302:PO4:O4	2.00	0.44
1:I:179:LYS:HB2	1:I:179:LYS:HE2	1.73	0.44
1:B:41:VAL:HG22	1:B:48:VAL:HG12	2.00	0.44
1:J:139:LYS:HE2	1:J:181:ASN:HD21	1.81	0.44
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.53	0.44
1:G:152:VAL:HG12	1:G:195:VAL:HG23	2.00	0.44
1:A:-2:ASP:CB	1:E:24:ASP:HA	2.48	0.43
1:G:145:HIS:HE1	2:G:302:PO4:O4	2.00	0.43
1:D:19:ILE:HD12	1:D:21:THR:HG23	2.00	0.43
1:I:180:LYS:HG2	1:I:181:ASN:N	2.33	0.43
1:I:157:GLU:HG2	1:I:158:ASN:H	1.83	0.43
1:H:125:VAL:O	1:H:125:VAL:HG12	2.18	0.43
3:J:302:4P6:C3	3:J:302:4P6:H26	2.49	0.43
1:G:70:SER:HB2	1:G:71:PRO:CD	2.48	0.43
1:G:130:THR:HG22	1:G:133:GLY:H	1.84	0.43
1:I:152:VAL:HG12	1:I:195:VAL:CG2	2.49	0.43
1:E:41:VAL:CG1	1:E:125:VAL:HG11	2.48	0.43
1:H:145:HIS:HE1	2:I:301:PO4:O2	2.02	0.43
1:F:145:HIS:HE1	2:G:301:PO4:O1	2.00	0.43
1:I:55:GLN:HA	1:I:114:MET:HG3	2.01	0.43
1:F:161:ASP:HB2	1:F:164:TYR:HD2	1.84	0.42
1:C:41:VAL:CG1	1:C:125:VAL:HG11	2.50	0.42
1:F:149:GLU:OE2	1:G:3:ARG:NH2	2.38	0.42
3:E:301:4P6:H26	3:E:301:4P6:C3	2.47	0.42
1:F:145:HIS:HB2	1:F:150:ILE:HD12	2.01	0.42
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.55	0.42
1:C:153:ASP:HA	1:C:154:PRO:HD3	1.88	0.42
1:I:41:VAL:CG1	1:I:125:VAL:HG11	2.49	0.42
1:C:41:VAL:CG1	1:C:125:VAL:CG1	2.98	0.42
1:F:125:VAL:HG12	1:F:125:VAL:O	2.18	0.42
1:B:131:GLU:O	1:B:202:ARG:NH1	2.50	0.42
1:B:188:CYS:HA	1:B:189:PRO:HD3	1.86	0.42
1:J:152:VAL:O	1:J:152:VAL:HG23	2.20	0.42
1:B:32:SER:HA	1:B:178:GLN:OE1	2.19	0.42
1:C:145:HIS:HE1	2:C:301:PO4:O2	2.02	0.42
1:I:32:SER:HA	1:I:178:GLN:HE22	1.85	0.42
1:C:70:SER:HB2	1:C:71:PRO:CD	2.50	0.41
1:B:192:TYR:OH	3:B:302:4P6:H21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:O	1:B:194:ASP:HB2	2.19	0.41
1:H:175:ASP:HB3	1:H:200[B]:ASN:HD22	1.85	0.41
1:F:172:GLU:OE2	1:F:202:ARG:NE	2.50	0.41
1:F:114:MET:CE	3:J:302:4P6:C12	2.98	0.41
1:D:151:SER:HB2	1:D:193:GLU:OE1	2.20	0.41
1:E:83:VAL:HG13	1:E:84:PRO:HD2	2.01	0.41
1:J:99:THR:HG23	1:J:116:SER:HB3	2.01	0.41
1:A:118:ARG:HH12	1:E:120:ARG:HH21	1.69	0.41
1:B:147:SER:CB	1:B:193:GLU:HG3	2.51	0.41
1:H:15:ARG:HD3	4:H:458:HOH:O	2.20	0.41
1:A:99:THR:HG23	1:A:116:SER:HB3	2.03	0.41
1:E:41:VAL:CG1	1:E:125:VAL:CG1	2.99	0.41
1:G:153:ASP:HA	1:G:154:PRO:HD3	1.88	0.41
1:I:167:GLN:HG2	4:I:457:HOH:O	2.21	0.41
1:B:70:SER:HB2	1:B:71:PRO:CD	2.50	0.40
1:B:77:PRO:HA	1:B:102:LEU:HD23	2.02	0.40
1:D:147:SER:HB3	1:D:193:GLU:HG3	2.04	0.40
1:A:67:SER:HA	1:A:70:SER:OG	2.20	0.40
1:D:184:THR:HG23	1:D:190:GLU:O	2.22	0.40
1:I:139:LYS:HG2	1:I:196:GLU:HG2	2.02	0.40
1:B:33:LEU:H	1:B:178:GLN:HE22	1.69	0.40
1:F:48:VAL:HG12	1:F:49:ASP:N	2.35	0.40
1:J:155:THR:OG1	1:J:156:THR:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/218 (96%)	208 (100%)	1 (0%)	0	100	100
1	B	209/218 (96%)	208 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	206/218 (94%)	206 (100%)	0	0	100	100
1	D	212/218 (97%)	211 (100%)	1 (0%)	0	100	100
1	E	208/218 (95%)	206 (99%)	2 (1%)	0	100	100
1	F	210/218 (96%)	208 (99%)	1 (0%)	1 (0%)	34	17
1	G	211/218 (97%)	209 (99%)	1 (0%)	1 (0%)	34	17
1	H	205/218 (94%)	205 (100%)	0	0	100	100
1	I	209/218 (96%)	207 (99%)	2 (1%)	0	100	100
1	J	209/218 (96%)	207 (99%)	2 (1%)	0	100	100
All	All	2088/2180 (96%)	2075 (99%)	11 (0%)	2 (0%)	56	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	161	ASP
1	G	189	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/204 (95%)	191 (99%)	2 (1%)	82	76
1	B	191/204 (94%)	188 (98%)	3 (2%)	70	57
1	C	188/204 (92%)	186 (99%)	2 (1%)	80	72
1	D	191/204 (94%)	189 (99%)	2 (1%)	82	76
1	E	186/204 (91%)	185 (100%)	1 (0%)	92	90
1	F	189/204 (93%)	188 (100%)	1 (0%)	92	90
1	G	191/204 (94%)	190 (100%)	1 (0%)	92	90
1	H	191/204 (94%)	191 (100%)	0	100	100
1	I	187/204 (92%)	184 (98%)	3 (2%)	70	57
1	J	192/204 (94%)	190 (99%)	2 (1%)	82	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1899/2040 (93%)	1882 (99%)	17 (1%)	84	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASP
1	A	161	ASP
1	B	24	ASP
1	B	55	GLN
1	B	61	ARG
1	C	181	ASN
1	C	188	CYS
1	D	112	LEU
1	D	122	SER
1	E	151	SER
1	F	24	ASP
1	G	130	THR
1	I	59	SER
1	I	183	VAL
1	I	186	SER
1	J	24	ASP
1	J	180	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	200	ASN
1	F	181	ASN
1	G	200	ASN
1	J	181	ASN

### 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 carbohydrates 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	$\# Z  > 2$
2	PO4	A	301	-	4,4,4	0.41	0	6,6,6	0.28	0
2	PO4	A	302	-	4,4,4	0.39	0	6,6,6	0.28	0
3	4P6	A	303	-	19,20,20	0.65	0	19,26,26	1.71	6 (31%)
2	PO4	B	301	-	4,4,4	0.39	0	6,6,6	0.25	0
3	4P6	B	302	-	19,20,20	0.52	0	19,26,26	1.68	4 (21%)
2	PO4	C	301	-	4,4,4	0.37	0	6,6,6	0.27	0
3	4P6	C	302	-	19,20,20	0.53	0	19,26,26	1.83	5 (26%)
2	PO4	D	301	-	4,4,4	0.44	0	6,6,6	0.25	0
3	4P6	D	302	-	19,20,20	0.59	0	19,26,26	1.73	7 (36%)
3	4P6	E	301	-	19,20,20	0.51	0	19,26,26	1.56	4 (21%)
3	4P6	F	301	-	19,20,20	0.59	0	19,26,26	1.76	6 (31%)
2	PO4	G	301	-	4,4,4	0.37	0	6,6,6	0.26	0
2	PO4	G	302	-	4,4,4	0.42	0	6,6,6	0.28	0
3	4P6	G	303	-	19,20,20	0.62	0	19,26,26	1.89	5 (26%)
3	4P6	H	301	-	19,20,20	0.43	0	19,26,26	1.65	5 (26%)
2	PO4	I	301	-	4,4,4	0.54	0	6,6,6	0.29	0
2	PO4	I	302	-	4,4,4	0.43	0	6,6,6	0.29	0
3	4P6	I	303	-	19,20,20	0.59	0	19,26,26	2.15	4 (21%)
2	PO4	J	301	-	4,4,4	0.32	0	6,6,6	0.27	0
3	4P6	J	302	-	19,20,20	0.59	0	19,26,26	1.56	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
2	PO4	A	301	-	-	0/0/0/0	0/0/0/0
2	PO4	A	302	-	-	0/0/0/0	0/0/0/0
3	4P6	A	303	-	-	0/6/19/19	0/2/3/3
2	PO4	B	301	-	-	0/0/0/0	0/0/0/0
3	4P6	B	302	-	-	0/6/19/19	0/2/3/3
2	PO4	C	301	-	-	0/0/0/0	0/0/0/0
3	4P6	C	302	-	-	0/6/19/19	0/2/3/3
2	PO4	D	301	-	-	0/0/0/0	0/0/0/0
3	4P6	D	302	-	-	0/6/19/19	0/2/3/3
3	4P6	E	301	-	-	0/6/19/19	0/2/3/3
3	4P6	F	301	-	-	0/6/19/19	0/2/3/3
2	PO4	G	301	-	-	0/0/0/0	0/0/0/0
2	PO4	G	302	-	-	0/0/0/0	0/0/0/0
3	4P6	G	303	-	-	0/6/19/19	0/2/3/3
3	4P6	H	301	-	-	0/6/19/19	0/2/3/3
2	PO4	I	301	-	-	0/0/0/0	0/0/0/0
2	PO4	I	302	-	-	0/0/0/0	0/0/0/0
3	4P6	I	303	-	-	0/6/19/19	0/2/3/3
2	PO4	J	301	-	-	0/0/0/0	0/0/0/0
3	4P6	J	302	-	-	0/6/19/19	0/2/3/3

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	4P6	C12-C11-C10	-3.61	113.58	119.89
3	F	301	4P6	C12-C11-C10	-3.48	113.81	119.89
3	G	303	4P6	C2-C7-S18	-3.46	109.40	113.23
3	E	301	4P6	C12-C11-C10	-3.45	113.87	119.89
3	D	302	4P6	C12-C11-C10	-3.38	113.99	119.89
3	I	303	4P6	C2-C7-S18	-3.38	109.49	113.23
3	C	302	4P6	C12-C11-C10	-3.30	114.13	119.89
3	J	302	4P6	C12-C11-C10	-3.23	114.24	119.89
3	H	301	4P6	C12-C11-C10	-3.23	114.25	119.89
3	A	303	4P6	C1-C3-C8	-2.73	116.90	120.33
3	C	302	4P6	C2-C7-S18	-2.73	110.21	113.23
3	I	303	4P6	C12-C11-C10	-2.72	115.14	119.89
3	D	302	4P6	C1-C3-C8	-2.70	116.94	120.33
3	F	301	4P6	C2-C7-S18	-2.63	110.32	113.23
3	A	303	4P6	C8-C10-C11	-2.59	119.39	122.46
3	A	303	4P6	C2-C7-S18	-2.55	110.41	113.23
3	F	301	4P6	C8-C10-C11	-2.51	119.49	122.46
3	D	302	4P6	C14-C13-C11	-2.42	107.47	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	301	4P6	C1-C3-C8	-2.40	117.31	120.33
3	G	303	4P6	C14-C13-C11	-2.39	107.53	112.28
3	G	303	4P6	C8-C10-C11	-2.38	119.63	122.46
3	J	302	4P6	C14-C13-C11	-2.37	107.58	112.28
3	D	302	4P6	C8-C10-C11	-2.36	119.66	122.46
3	E	301	4P6	C2-C7-S18	-2.35	110.63	113.23
3	H	301	4P6	C2-C7-S18	-2.35	110.63	113.23
3	I	303	4P6	C4-C9-S18	-2.35	108.27	110.92
3	B	302	4P6	C8-C10-C11	-2.33	119.70	122.46
3	B	302	4P6	C2-C7-S18	-2.31	110.67	113.23
3	A	303	4P6	C12-C11-C10	-2.29	115.90	119.89
3	J	302	4P6	C1-C3-C8	-2.28	117.47	120.33
3	F	301	4P6	C14-C13-C11	-2.17	107.98	112.28
3	G	303	4P6	C12-C11-C10	-2.15	116.13	119.89
3	C	302	4P6	C1-C3-C8	-2.14	117.64	120.33
3	D	302	4P6	C2-C7-S18	-2.07	110.94	113.23
3	J	302	4P6	C2-C7-S18	-2.05	110.97	113.23
3	F	301	4P6	C1-C3-C8	-2.04	117.77	120.33
3	H	301	4P6	C3-C8-C10	2.03	124.31	120.72
3	D	302	4P6	C7-S18-C9	2.07	92.89	91.90
3	J	302	4P6	C7-S18-C9	2.11	92.91	91.90
3	J	302	4P6	C3-C8-C6	2.13	120.16	117.67
3	A	303	4P6	C3-C8-C6	2.45	120.54	117.67
3	D	302	4P6	C3-C8-C6	2.50	120.60	117.67
3	E	301	4P6	C13-C11-C12	2.80	128.12	125.21
3	E	301	4P6	C7-S18-C9	2.88	93.27	91.90
3	F	301	4P6	C7-S18-C9	3.16	93.41	91.90
3	H	301	4P6	C7-S18-C9	3.18	93.42	91.90
3	B	302	4P6	C7-S18-C9	3.31	93.48	91.90
3	A	303	4P6	C7-S18-C9	3.56	93.60	91.90
3	C	302	4P6	C3-C8-C10	3.65	127.19	120.72
3	C	302	4P6	C7-S18-C9	3.69	93.66	91.90
3	G	303	4P6	C7-S18-C9	5.01	94.30	91.90
3	I	303	4P6	C7-S18-C9	6.52	95.02	91.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 33 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PO4	1	0
2	A	302	PO4	1	0
3	A	303	4P6	3	0
3	B	302	4P6	4	0
2	C	301	PO4	1	0
3	D	302	4P6	3	0
3	E	301	4P6	6	0
3	F	301	4P6	2	0
2	G	301	PO4	1	0
2	G	302	PO4	1	0
3	G	303	4P6	1	0
3	H	301	4P6	1	0
2	I	301	PO4	1	0
2	I	302	PO4	1	0
3	I	303	4P6	3	0
3	J	302	4P6	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	212/218 (97%)	-0.25	2 (0%) 85 85	18, 27, 40, 49	0
1	B	210/218 (96%)	-0.31	3 (1%) 78 78	16, 24, 37, 51	0
1	C	209/218 (95%)	-0.30	0 100 100	16, 24, 43, 62	0
1	D	214/218 (98%)	-0.29	1 (0%) 91 91	15, 24, 40, 51	0
1	E	212/218 (97%)	-0.27	0 100 100	19, 26, 49, 63	0
1	F	214/218 (98%)	-0.21	1 (0%) 91 91	16, 25, 43, 51	0
1	G	214/218 (98%)	-0.28	1 (0%) 91 91	15, 25, 44, 65	0
1	H	208/218 (95%)	-0.23	5 (2%) 62 60	16, 22, 41, 61	0
1	I	211/218 (96%)	-0.33	0 100 100	15, 24, 42, 57	0
1	J	211/218 (96%)	-0.34	4 (1%) 70 69	14, 23, 38, 53	0
All	All	2115/2180 (97%)	-0.28	17 (0%) 87 87	14, 24, 42, 65	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-6	TYR	4.1
1	H	-3	ASP	2.9
1	H	23	ARG	2.8
1	G	158	ASN	2.7
1	J	24	ASP	2.7
1	A	207	SER	2.6
1	H	-4	ASP	2.5
1	B	23	ARG	2.3
1	F	155	THR	2.3
1	H	-2	ASP	2.2
1	J	152	VAL	2.2
1	A	24	ASP	2.1
1	J	205	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	-1	ASP	2.0
1	B	-4	ASP	2.0
1	B	68	SER	2.0
1	J	-4	ASP	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	G	301	5/5	0.99	0.12	1.54	17,18,19,22	0
3	4P6	C	302	18/18	0.89	0.13	0.63	19,32,40,46	0
2	PO4	D	301	5/5	0.99	0.07	-0.02	18,19,20,21	0
3	4P6	G	303	18/18	0.93	0.09	-0.10	19,28,37,43	0
2	PO4	A	302	5/5	0.99	0.07	-0.16	18,20,22,23	0
2	PO4	G	302	5/5	0.99	0.07	-0.27	18,18,21,21	0
3	4P6	I	303	18/18	0.95	0.09	-0.28	18,27,36,39	0
3	4P6	E	301	18/18	0.92	0.09	-0.40	24,32,39,40	0
3	4P6	D	302	18/18	0.94	0.08	-0.43	22,30,39,41	0
2	PO4	I	301	5/5	0.99	0.07	-0.44	17,18,18,19	0
3	4P6	A	303	18/18	0.93	0.08	-0.49	20,30,37,41	0
3	4P6	B	302	18/18	0.94	0.08	-0.57	17,26,35,39	0
3	4P6	F	301	18/18	0.93	0.09	-0.58	19,31,38,44	0
2	PO4	B	301	5/5	0.99	0.08	-0.72	16,16,17,17	0
2	PO4	C	301	5/5	0.99	0.07	-0.72	17,17,19,20	0
3	4P6	J	302	18/18	0.95	0.08	-0.77	17,29,37,43	0
3	4P6	H	301	18/18	0.97	0.07	-0.94	16,24,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	301	5/5	0.99	0.05	-1.41	21,21,23,25	0
2	PO4	I	302	5/5	0.98	0.06	-1.65	20,20,21,24	0
2	PO4	J	301	5/5	0.99	0.06	-2.46	20,20,20,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.