



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:32 pm GMT

PDB ID : 1TZY  
Title : Crystal Structure of the Core-Histone Octamer to 1.90 Angstrom Resolution  
Authors : Wood, C.M.; Nicholson, J.M.; Chantalat, L.; Reynolds, C.D.; Lambert, S.J.;  
Baldwin, J.P.  
Deposited on : 2004-07-12  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

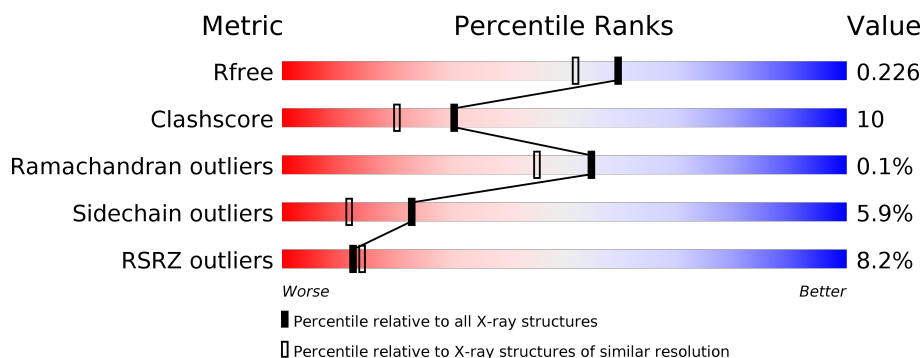
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	129	<div> <div>6%</div> <div>68% 12% 18%</div> </div>
1	E	129	<div> <div>5%</div> <div>61% 16% 19%</div> </div>
2	B	126	<div> <div>6%</div> <div>59% 11% 27%</div> </div>
2	F	126	<div> <div>8%</div> <div>64% 10% 26%</div> </div>
3	C	136	<div> <div>7%</div> <div>56% 11% 30%</div> </div>
3	G	136	<div> <div>10%</div> <div>53% 15% 28%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	103	
4	H	103	

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
5	PO4	B	1502	-	-	X	X
5	PO4	C	1505	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6625 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H2A-IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	0	0	0
			815	516	158	141			
1	E	104	Total	C	N	O	0	0	0
			797	504	154	139			

- Molecule 2 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			720	453	129	136	2			
2	F	93	Total	C	N	O	S	0	0	0
			724	455	130	137	2			

- Molecule 3 is a protein called HISTONE H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			767	486	141	137	3			
3	G	98	Total	C	N	O	S	0	0	0
			807	508	156	140	3			

- Molecule 4 is a protein called HISTONE H4-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
4	H	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	4	Total	Cl	0	0
			4	4		
6	D	3	Total	Cl	0	0
			3	3		
6	E	2	Total	Cl	0	0
			2	2		
6	H	3	Total	Cl	0	0
			3	3		
6	B	2	Total	Cl	0	0
			2	2		
6	C	3	Total	Cl	0	0
			3	3		
6	A	4	Total	Cl	0	0
			4	4		

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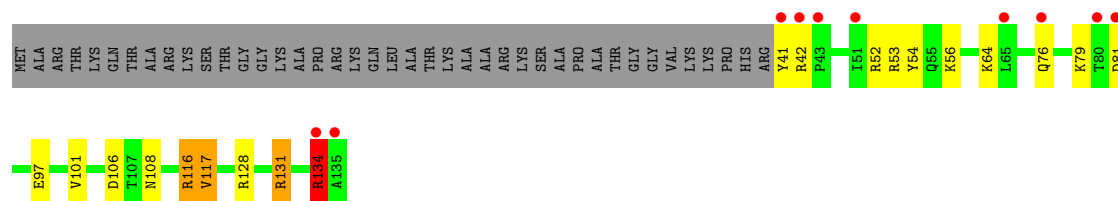
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Cl	0	0
			2	2		

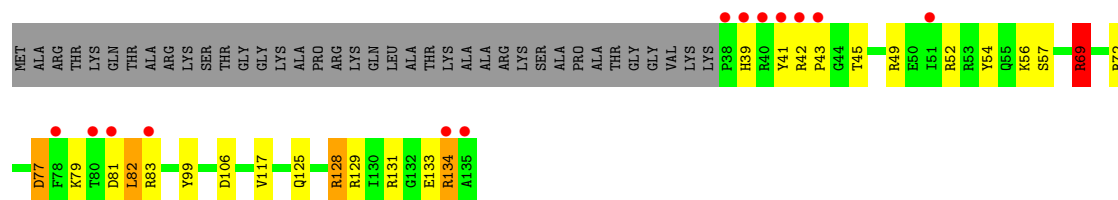
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total	O	0	0
			94	94		
7	B	83	Total	O	0	0
			83	83		
7	C	66	Total	O	0	0
			66	66		
7	D	75	Total	O	0	0
			75	75		
7	E	86	Total	O	0	0
			86	86		
7	F	69	Total	O	0	0
			69	69		
7	G	80	Total	O	0	0
			80	80		
7	H	59	Total	O	0	0
			59	59		

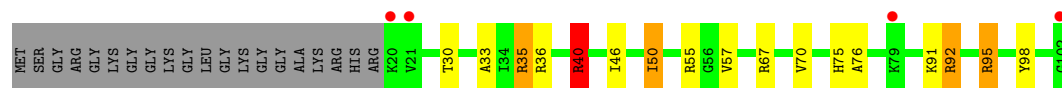




• Molecule 3: HISTONE H3



• Molecule 4: HISTONE H4-VI



• Molecule 4: HISTONE H4-VI





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.35Å 158.35Å 103.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.96 – 1.90 14.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (14.96-1.90) 99.9 (14.95-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.187 , 0.222 0.192 , 0.226	Depositor DCC
$R_{free}$ test set	5806 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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, CL

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	1.03	0/825	1.52	12/1112 (1.1%)
1	E	0.99	0/807	1.28	8/1090 (0.7%)
2	B	1.08	0/731	0.95	2/983 (0.2%)
2	F	1.02	0/735	0.87	1/987 (0.1%)
3	C	1.11	0/777	1.56	7/1043 (0.7%)
3	G	1.13	1/819 (0.1%)	1.44	15/1097 (1.4%)
4	D	1.25	4/669 (0.6%)	1.45	8/894 (0.9%)
4	H	1.14	0/680	1.57	12/908 (1.3%)
All	All	1.09	5/6043 (0.1%)	1.35	65/8114 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	2
3	G	0	1
4	D	1	0
All	All	1	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	35	ARG	CZ-NH1	6.64	1.41	1.33
4	D	70	VAL	CB-CG2	-6.09	1.40	1.52
4	D	98	TYR	CD2-CE2	-5.28	1.31	1.39
4	D	35	ARG	CG-CD	5.08	1.64	1.51
3	G	99	TYR	CD2-CE2	-5.04	1.31	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	116	ARG	NE-CZ-NH2	-24.73	107.94	120.30
3	G	69	ARG	NE-CZ-NH1	-23.13	108.73	120.30
1	A	32	ARG	NE-CZ-NH1	22.95	131.78	120.30
4	H	40	ARG	NE-CZ-NH1	21.41	131.01	120.30
1	A	32	ARG	NE-CZ-NH2	-20.00	110.30	120.30
1	E	88	ARG	NE-CZ-NH2	20.00	130.30	120.30
4	H	40	ARG	NE-CZ-NH2	-19.39	110.60	120.30
3	C	131	ARG	NE-CZ-NH2	18.57	129.59	120.30
3	C	131	ARG	NE-CZ-NH1	-16.10	112.25	120.30
1	A	88	ARG	NE-CZ-NH1	-16.02	112.29	120.30
1	E	88	ARG	NE-CZ-NH1	-15.95	112.32	120.30
3	G	69	ARG	NE-CZ-NH2	15.30	127.95	120.30
1	A	88	ARG	NE-CZ-NH2	14.75	127.68	120.30
3	C	116	ARG	NE-CZ-NH1	14.38	127.49	120.30
4	D	35	ARG	NE-CZ-NH2	-14.05	113.28	120.30
4	D	40	ARG	NE-CZ-NH2	-13.80	113.40	120.30
4	D	40	ARG	NE-CZ-NH1	13.39	127.00	120.30
4	D	35	ARG	NE-CZ-NH1	11.97	126.29	120.30
4	H	78	ARG	NE-CZ-NH1	-11.22	114.69	120.30
3	C	116	ARG	CD-NE-CZ	10.44	138.22	123.60
1	A	32	ARG	CB-CG-CD	9.54	136.40	111.60
4	H	78	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	32	ARG	CD-NE-CZ	9.05	136.27	123.60
1	E	72	ASP	CB-CG-OD2	8.41	125.87	118.30
3	G	69	ARG	CD-NE-CZ	8.26	135.17	123.60
3	G	128	ARG	NE-CZ-NH2	-7.97	116.31	120.30
3	G	131	ARG	NE-CZ-NH2	-7.57	116.52	120.30
4	H	40	ARG	CD-NE-CZ	7.42	133.99	123.60
4	H	95	ARG	NE-CZ-NH1	-7.29	116.65	120.30
4	H	95	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	E	29	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	88	ARG	CB-CG-CD	7.10	130.06	111.60
4	D	95	ARG	NE-CZ-NH1	-7.07	116.76	120.30
1	E	88	ARG	CD-NE-CZ	6.97	133.36	123.60
1	E	17	ARG	NE-CZ-NH2	6.68	123.64	120.30
3	G	128	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	E	88	ARG	CB-CG-CD	6.37	128.16	111.60
1	A	88	ARG	CD-NE-CZ	6.30	132.41	123.60
1	A	72	ASP	CB-CG-OD2	6.27	123.94	118.30
4	H	23	ARG	NE-CZ-NH1	6.23	123.41	120.30
3	G	69	ARG	CG-CD-NE	-6.17	98.85	111.80
4	H	93	GLN	CA-CB-CG	6.14	126.91	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	106	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	51	ASP	CB-CG-OD1	6.00	123.70	118.30
3	G	77	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	90	ASP	CB-CG-OD2	5.86	123.57	118.30
3	G	81	ASP	CB-CG-OD2	5.83	123.55	118.30
3	G	52	ARG	NE-CZ-NH2	5.58	123.09	120.30
3	C	81	ASP	CB-CG-OD2	5.57	123.31	118.30
4	H	93	GLN	CB-CA-C	-5.47	99.45	110.40
1	A	17	ARG	NE-CZ-NH1	-5.46	117.57	120.30
4	D	57	VAL	CG1-CB-CG2	5.45	119.62	110.90
4	D	36	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	C	131	ARG	CD-NE-CZ	5.38	131.13	123.60
3	G	52	ARG	NE-CZ-NH1	-5.27	117.67	120.30
3	G	134	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	G	131	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	F	106	LEU	CA-CB-CG	5.20	127.25	115.30
4	H	24	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	88	ARG	CA-CB-CG	5.17	124.78	113.40
3	G	72	ARG	NE-CZ-NH2	5.17	122.89	120.30
4	D	55	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	E	29	ARG	NE-CZ-NH1	-5.04	117.78	120.30
2	B	51	ASP	OD1-CG-OD2	-5.02	113.77	123.30
4	H	39	ARG	NE-CZ-NH2	5.01	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	30	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	123	SER	Peptide
3	C	116	ARG	Sidechain
3	C	134	ARG	Peptide
3	G	69	ARG	Sidechain

## 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	815	0	877	16	0
1	E	797	0	851	24	0
2	B	720	0	740	18	0
2	F	724	0	738	11	0
3	C	767	0	791	19	0
3	G	807	0	844	23	0
4	D	662	0	709	21	0
4	H	673	0	722	14	0
5	A	5	0	0	1	0
5	B	5	0	0	3	0
5	C	5	0	0	3	0
5	E	10	0	0	1	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
6	C	3	0	0	1	0
6	D	3	0	0	1	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	4	0	0	1	0
6	H	3	0	0	1	0
7	A	94	0	0	4	0
7	B	83	0	0	7	0
7	C	66	0	0	6	0
7	D	75	0	0	9	0
7	E	86	0	0	6	0
7	F	69	0	0	4	0
7	G	80	0	0	7	0
7	H	59	0	0	7	0
All	All	6625	0	6272	129	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 10.

All (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:ARG:HD2	5:C:1505:PO4:O3	1.57	1.03
3:C:53:ARG:CD	5:C:1505:PO4:O3	2.18	0.92
3:C:101:VAL:HB	7:D:1691:HOH:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:HIS:HB3	2:B:52:THR:HG23	1.52	0.91
2:B:33:ARG:HA	7:B:1654:HOH:O	1.74	0.87
3:G:83:ARG:HD3	7:G:1654:HOH:O	1.75	0.86
1:E:73:ASN:HB3	7:E:1705:HOH:O	1.76	0.86
3:G:54:TYR:O	4:H:40:ARG:HD3	1.76	0.84
3:C:56:LYS:HE2	7:C:1651:HOH:O	1.75	0.84
3:C:54:TYR:O	4:D:40:ARG:HD3	1.77	0.83
3:G:125:GLN:HA	3:G:134:ARG:NH1	1.94	0.81
1:A:32:ARG:HD3	5:A:1501:PO4:O2	1.81	0.80
1:A:84:GLN:OE1	1:A:88:ARG:HD3	1.84	0.77
4:H:19:ARG:HB3	7:H:1671:HOH:O	1.84	0.76
4:H:46:ILE:HG23	4:H:50:ILE:HG12	1.67	0.76
4:H:78:ARG:HD2	7:H:1675:HOH:O	1.84	0.75
4:H:46:ILE:CG2	4:H:50:ILE:HG12	2.16	0.75
3:G:128:ARG:HB2	3:G:134:ARG:HH11	1.51	0.74
3:G:54:TYR:O	4:H:40:ARG:CD	2.35	0.74
3:G:128:ARG:HB2	3:G:134:ARG:NH1	2.03	0.72
3:C:52:ARG:O	3:C:56:LYS:HG2	1.89	0.72
1:A:38:ASN:HA	7:A:1687:HOH:O	1.90	0.71
3:G:128:ARG:NH2	3:G:133:GLU:OE1	2.23	0.71
3:G:69:ARG:HD3	6:G:1611:CL:CL	2.27	0.70
3:C:54:TYR:O	4:D:40:ARG:CD	2.39	0.70
1:E:117:PRO:C	7:E:1693:HOH:O	2.29	0.70
1:E:73:ASN:ND2	7:E:1699:HOH:O	2.27	0.67
3:C:64:LYS:HD2	7:C:1674:HOH:O	1.93	0.66
4:D:30:THR:HG21	6:D:1612:CL:CL	2.31	0.66
4:D:30:THR:HG23	4:D:33:ALA:H	1.59	0.66
3:C:117:VAL:HG22	1:E:115:LEU:CD2	2.24	0.66
1:E:84:GLN:OE1	1:E:88:ARG:HD3	1.97	0.65
3:G:79:LYS:HB3	3:G:82:LEU:HD22	1.78	0.65
3:G:41:TYR:CZ	3:G:49:ARG:NH2	2.67	0.63
3:C:97:GLU:O	3:C:101:VAL:HG22	1.99	0.62
2:B:51:ASP:HA	7:B:1627:HOH:O	1.98	0.61
1:E:29:ARG:HD2	2:F:35:GLU:OE2	2.00	0.61
1:E:17:ARG:HG3	1:E:17:ARG:HH21	1.66	0.61
4:D:46:ILE:HG23	4:D:50:ILE:HG12	1.82	0.61
3:C:134:ARG:HB2	7:C:1669:HOH:O	2.01	0.60
2:F:34:LYS:HA	7:F:1659:HOH:O	2.01	0.60
3:G:128:ARG:HD3	3:G:134:ARG:HH12	1.67	0.60
7:A:1630:HOH:O	2:B:113:GLU:HG2	2.01	0.59
1:E:31:HIS:HD2	7:E:1644:HOH:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79:LYS:HA	7:G:1652:HOH:O	2.02	0.58
1:E:64:GLU:O	2:F:49:HIS:HE1	1.85	0.58
2:B:35:GLU:HB3	2:B:67:ASN:HD21	1.69	0.58
4:D:35:ARG:HD3	7:D:1689:HOH:O	2.03	0.58
1:A:79:ILE:H	1:A:82:HIS:CD2	2.22	0.57
3:C:53:ARG:HD3	5:C:1505:PO4:O3	2.02	0.57
1:E:84:GLN:CD	1:E:88:ARG:HD3	2.24	0.57
7:A:1712:HOH:O	2:B:52:THR:HG21	2.04	0.57
2:B:96:THR:OG1	4:D:75:HIS:HD2	1.86	0.57
3:C:79:LYS:CG	7:D:1682:HOH:O	2.53	0.56
1:A:115:LEU:CD2	3:G:117:VAL:HG22	2.36	0.56
4:H:19:ARG:HD3	7:H:1671:HOH:O	2.06	0.56
3:G:57:SER:OG	7:G:1690:HOH:O	2.17	0.56
1:A:64:GLU:HB2	2:B:48:VAL:HG21	1.88	0.56
1:A:78:ILE:HA	1:A:82:HIS:HD2	1.70	0.56
5:E:1504:PO4:O1	7:E:1704:HOH:O	2.18	0.56
4:D:67:ARG:CD	7:D:1645:HOH:O	2.54	0.56
1:E:79:ILE:H	1:E:82:HIS:CD2	2.24	0.55
3:G:56:LYS:HE2	7:G:1662:HOH:O	2.06	0.55
4:D:67:ARG:HD3	7:D:1645:HOH:O	2.07	0.55
4:D:50:ILE:O	4:D:50:ILE:HD12	2.06	0.55
1:A:84:GLN:CD	1:A:88:ARG:HD3	2.27	0.54
7:B:1637:HOH:O	4:D:75:HIS:HE1	1.91	0.53
3:G:41:TYR:HB3	7:G:1640:HOH:O	2.08	0.53
3:G:57:SER:CB	7:G:1690:HOH:O	2.56	0.53
4:D:50:ILE:HD12	4:D:50:ILE:C	2.30	0.52
1:E:14:ALA:HA	1:E:19:SER:HB3	1.91	0.52
2:F:33:ARG:HA	7:F:1667:HOH:O	2.09	0.52
4:H:59:LYS:CE	7:H:1655:HOH:O	2.58	0.52
4:H:59:LYS:HE2	7:H:1655:HOH:O	2.09	0.52
2:B:39:ILE:HG12	7:B:1623:HOH:O	2.10	0.51
1:A:114:VAL:O	1:A:114:VAL:HG12	2.09	0.50
2:B:51:ASP:OD2	2:B:51:ASP:N	2.43	0.50
2:B:84:ASN:HD21	4:D:76:ALA:HB2	1.77	0.49
4:D:91:LYS:NZ	7:D:1680:HOH:O	2.41	0.49
3:G:57:SER:HB2	7:G:1690:HOH:O	2.12	0.49
3:G:54:TYR:O	4:H:40:ARG:HD2	2.13	0.48
4:D:92:ARG:HB3	4:D:92:ARG:CZ	2.43	0.48
1:E:17:ARG:HG3	1:E:17:ARG:NH2	2.24	0.47
3:C:128:ARG:HD3	6:C:1619:CL:CL	2.51	0.47
2:B:33:ARG:HB2	7:B:1678:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:GLY:O	1:E:38:ASN:HB2	2.14	0.47
1:A:84:GLN:OE1	1:A:88:ARG:CD	2.60	0.47
2:B:50:PRO:HD2	2:B:51:ASP:OD2	2.14	0.47
1:E:79:ILE:H	1:E:82:HIS:HD2	1.60	0.47
2:F:33:ARG:HD2	2:F:33:ARG:O	2.14	0.46
3:G:45:THR:O	3:G:49:ARG:HG3	2.15	0.46
4:D:91:LYS:HD3	7:D:1680:HOH:O	2.15	0.46
1:A:38:ASN:HB3	7:A:1646:HOH:O	2.16	0.45
1:E:78:ILE:HA	1:E:82:HIS:HD2	1.82	0.45
3:C:42:ARG:HG2	7:C:1678:HOH:O	2.16	0.45
3:C:117:VAL:HG22	1:E:115:LEU:HD23	1.97	0.45
1:A:79:ILE:HG22	5:B:1502:PO4:O2	2.17	0.45
1:E:29:ARG:HH21	2:F:35:GLU:CD	2.20	0.45
1:A:88:ARG:HH11	1:A:94:ASN:ND2	2.14	0.44
2:F:124:SER:HA	7:F:1691:HOH:O	2.16	0.44
1:A:104:GLN:HG3	7:B:1690:HOH:O	2.16	0.44
1:E:36:LYS:CG	7:E:1684:HOH:O	2.66	0.44
4:H:95:ARG:NH1	6:H:1605:CL:CL	2.87	0.44
2:B:33:ARG:HD3	2:F:85:LYS:NZ	2.32	0.44
4:D:95:ARG:HD2	7:D:1632:HOH:O	2.18	0.44
4:H:93:GLN:HG2	7:H:1624:HOH:O	2.16	0.44
1:A:32:ARG:HG3	1:A:32:ARG:O	2.16	0.44
4:D:30:THR:CG2	4:D:33:ALA:H	2.30	0.44
2:B:57:LYS:HB2	5:B:1502:PO4:O3	2.18	0.43
1:E:47:ALA:N	1:E:48:PRO:HD2	2.34	0.43
3:C:101:VAL:HG23	7:C:1631:HOH:O	2.16	0.43
3:C:106:ASP:OD2	3:C:131:ARG:HD2	2.17	0.43
4:H:70:VAL:HG23	7:H:1637:HOH:O	2.17	0.43
4:D:46:ILE:CG2	4:D:50:ILE:HG12	2.46	0.43
2:B:50:PRO:HG3	7:B:1695:HOH:O	2.18	0.42
3:C:42:ARG:CG	7:C:1678:HOH:O	2.67	0.42
2:B:96:THR:OG1	4:D:75:HIS:CD2	2.71	0.42
1:E:92:GLU:OE2	1:E:95:LYS:NZ	2.53	0.42
1:E:88:ARG:HH11	1:E:94:ASN:ND2	2.16	0.42
4:D:67:ARG:HD2	7:D:1645:HOH:O	2.15	0.42
3:G:42:ARG:HB3	3:G:43:PRO:HD2	2.01	0.42
3:G:128:ARG:HD3	3:G:134:ARG:NH1	2.33	0.41
1:A:79:ILE:HB	5:B:1502:PO4:O2	2.21	0.41
2:F:84:ASN:HD21	4:H:76:ALA:HB2	1.85	0.41
2:B:70:PHE:CD1	2:B:70:PHE:C	2.93	0.41
3:G:79:LYS:HD3	3:G:82:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ARG:NH2	2:F:35:GLU:OE1	2.54	0.41
1:E:37:GLY:O	1:E:38:ASN:CB	2.65	0.41
2:F:39:ILE:HG23	7:F:1662:HOH:O	2.20	0.41

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	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
1	E	102/129 (79%)	98 (96%)	4 (4%)	0	100	100
2	B	90/126 (71%)	88 (98%)	2 (2%)	0	100	100
2	F	91/126 (72%)	89 (98%)	1 (1%)	1 (1%)	17	6
3	C	93/136 (68%)	93 (100%)	0	0	100	100
3	G	96/136 (71%)	92 (96%)	4 (4%)	0	100	100
4	D	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
4	H	82/103 (80%)	82 (100%)	0	0	100	100
All	All	739/988 (75%)	723 (98%)	15 (2%)	1 (0%)	55	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	123	SER

### 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	83/98 (85%)	77 (93%)	6 (7%)	17	7
1	E	81/98 (83%)	75 (93%)	6 (7%)	16	7
2	B	79/107 (74%)	72 (91%)	7 (9%)	11	4
2	F	78/107 (73%)	76 (97%)	2 (3%)	51	43
3	C	79/111 (71%)	74 (94%)	5 (6%)	21	10
3	G	85/111 (77%)	81 (95%)	4 (5%)	30	19
4	D	68/79 (86%)	65 (96%)	3 (4%)	33	22
4	H	69/79 (87%)	65 (94%)	4 (6%)	23	12
All	All	622/790 (79%)	585 (94%)	37 (6%)	23	12

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	19	SER
1	A	32	ARG
1	A	64	GLU
1	A	88	ARG
1	A	118	LYS
2	B	41	VAL
2	B	46	LYS
2	B	51	ASP
2	B	52	THR
2	B	57	LYS
2	B	113	GLU
2	B	124	SER
3	C	41	TYR
3	C	76	GLN
3	C	108	ASN
3	C	117	VAL
3	C	134	ARG
4	D	40	ARG
4	D	50	ILE
4	D	92	ARG
1	E	17	ARG
1	E	19	SER
1	E	24	GLN

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Mol	Chain	Res	Type
1	E	29	ARG
1	E	74	LYS
1	E	88	ARG
2	F	46	LYS
2	F	86	ARG
3	G	39	HIS
3	G	77	ASP
3	G	82	LEU
3	G	129	ARG
4	H	19	ARG
4	H	20	LYS
4	H	40	ARG
4	H	50	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	82	HIS
1	A	89	ASN
1	A	94	ASN
2	B	49	HIS
2	B	67	ASN
2	B	84	ASN
2	B	109	HIS
3	C	93	GLN
3	C	108	ASN
3	C	125	GLN
4	D	25	ASN
4	D	75	HIS
4	D	93	GLN
1	E	31	HIS
1	E	68	ASN
1	E	82	HIS
1	E	89	ASN
1	E	94	ASN
2	F	47	GLN
2	F	49	HIS
2	F	84	ASN
3	G	93	GLN
3	G	108	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 ⓘ

Of 28 ligands modelled in this entry, 23 are monoatomic - leaving 5 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	$\# Z  > 2$
5	PO4	A	1501	-	4,4,4	1.05	0	6,6,6	0.80	0
5	PO4	B	1502	-	4,4,4	1.03	0	6,6,6	1.52	1 (16%)
5	PO4	C	1505	-	4,4,4	0.65	0	6,6,6	0.74	0
5	PO4	E	1503	-	4,4,4	0.76	0	6,6,6	0.62	0
5	PO4	E	1504	-	4,4,4	0.80	0	6,6,6	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	A	1501	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1502	-	-	0/0/0/0	0/0/0/0
5	PO4	C	1505	-	-	0/0/0/0	0/0/0/0
5	PO4	E	1503	-	-	0/0/0/0	0/0/0/0
5	PO4	E	1504	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1502	PO4	O3-P-O1	-2.09	102.08	110.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1501	PO4	1	0
5	B	1502	PO4	3	0
5	C	1505	PO4	3	0
5	E	1504	PO4	1	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	106/129 (82%)	0.12	8 (7%)	15 17	32, 42, 72, 81	0
1	E	104/129 (80%)	0.20	7 (6%)	19 21	31, 43, 64, 79	0
2	B	92/126 (73%)	0.22	7 (7%)	15 16	31, 44, 62, 73	0
2	F	93/126 (73%)	0.25	10 (10%)	6 7	28, 41, 67, 86	0
3	C	95/136 (69%)	0.39	10 (10%)	7 8	32, 42, 72, 84	0
3	G	98/136 (72%)	0.57	13 (13%)	4 4	31, 41, 80, 90	0
4	D	83/103 (80%)	0.06	4 (4%)	31 35	31, 39, 62, 82	0
4	H	84/103 (81%)	0.08	3 (3%)	43 47	30, 39, 58, 79	0
All	All	755/988 (76%)	0.24	62 (8%)	12 14	28, 41, 69, 90	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	ALA	12.7
3	C	135	ALA	11.5
3	C	41	TYR	11.1
3	G	135	ALA	10.3
3	G	38	PRO	10.0
3	G	39	HIS	9.0
2	F	124	SER	8.6
2	F	125	LYS	8.3
4	H	19	ARG	7.6
1	A	118	LYS	7.6
3	G	41	TYR	7.5
4	D	21	VAL	7.4
4	D	102	GLY	6.3
3	G	40	ARG	5.8
1	A	13	LYS	5.4
4	D	20	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
3	G	81	ASP	4.8
3	G	42	ARG	4.5
2	B	33	ARG	4.4
4	H	102	GLY	4.2
1	E	42	ARG	4.2
3	G	134	ARG	4.0
3	C	81	ASP	3.8
2	F	33	ARG	3.6
1	A	71	ARG	3.6
3	G	80	THR	3.6
1	A	14	ALA	3.5
1	E	15	LYS	3.5
3	G	78	PHE	3.5
4	D	79	LYS	3.3
1	A	74	LYS	3.3
1	E	74	LYS	3.3
2	B	42	TYR	3.2
3	C	80	THR	3.2
2	F	42	TYR	3.1
3	G	83	ARG	2.9
3	C	134	ARG	2.9
3	G	43	PRO	2.8
1	E	41	GLU	2.8
4	H	79	LYS	2.7
2	B	51	ASP	2.6
2	B	124	SER	2.6
2	B	46	LYS	2.5
2	F	46	LYS	2.5
2	F	123	SER	2.5
2	B	123	SER	2.5
1	E	117	PRO	2.4
1	E	72	ASP	2.4
2	F	51	ASP	2.3
2	B	86	ARG	2.3
3	C	43	PRO	2.2
1	A	78	ILE	2.2
2	F	89	ILE	2.2
2	F	85	LYS	2.2
3	G	51	ILE	2.2
3	C	76	GLN	2.2
3	C	65	LEU	2.1
1	A	117	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	86	ARG	2.0
3	C	51	ILE	2.0
3	C	42	ARG	2.0
1	A	15	LYS	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
5	PO4	B	1502	5/5	0.94	0.57	10.15	50,65,70,70	0
6	CL	E	1621	1/1	0.93	0.15	1.11	68,68,68,68	0
6	CL	D	1617	1/1	0.99	0.10	0.09	46,46,46,46	0
6	CL	A	1604	1/1	0.99	0.08	0.01	38,38,38,38	0
6	CL	H	1605	1/1	0.99	0.09	-0.28	43,43,43,43	0
6	CL	E	1602	1/1	0.95	0.07	-0.56	46,46,46,46	0
6	CL	C	1619	1/1	0.98	0.05	-1.29	61,61,61,61	0
6	CL	B	1606	1/1	0.97	0.03	-1.31	41,41,41,41	0
6	CL	F	1616	1/1	0.97	0.04	-1.65	49,49,49,49	0
6	CL	G	1611	1/1	0.97	0.04	-2.13	51,51,51,51	0
6	CL	F	1623	1/1	0.99	0.04	-2.33	47,47,47,47	0
6	CL	B	1614	1/1	0.99	0.04	-3.20	44,44,44,44	0
6	CL	G	1608	1/1	0.97	0.07	-	48,48,48,48	0
6	CL	A	1613	1/1	0.91	0.25	-	71,71,71,71	0
6	CL	C	1615	1/1	0.96	0.11	-	49,49,49,49	0
6	CL	G	1601	1/1	0.98	0.08	-	45,45,45,45	0
6	CL	H	1618	1/1	0.98	0.20	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CL	A	1620	1/1	0.95	0.15	-	68,68,68,68	0
6	CL	G	1609	1/1	0.96	0.09	-	49,49,49,49	0
5	PO4	E	1504	5/5	0.92	0.29	-	83,86,87,89	0
6	CL	D	1603	1/1	0.98	0.06	-	45,45,45,45	0
5	PO4	A	1501	5/5	0.99	0.10	-	47,49,51,52	0
6	CL	A	1622	1/1	0.97	0.04	-	46,46,46,46	0
6	CL	H	1610	1/1	0.98	0.03	-	49,49,49,49	0
6	CL	C	1607	1/1	0.96	0.06	-	47,47,47,47	0
6	CL	D	1612	1/1	0.95	0.27	-	79,79,79,79	0
5	PO4	E	1503	5/5	0.94	0.42	-	85,85,87,88	0
5	PO4	C	1505	5/5	0.86	0.71	-	88,88,89,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.