



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:49 AM GMT

PDB ID : 2OBE  
Title : Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon  
Authors : Xue, F.; Rux, J.J.; Burnett, R.M.  
Deposited on : 2006-12-18  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

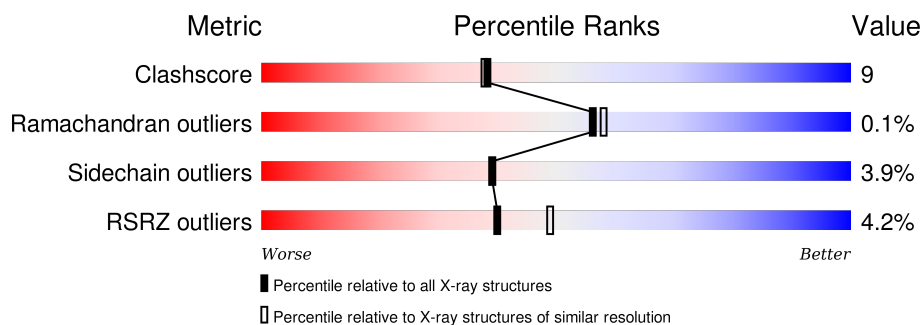
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	932	<div> <div>4%</div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
1	B	932	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	C	932	<div> <div>5%</div> <div>78%</div> <div>17%</div> <div>• •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2HP	A	1603	-	-	-	X
2	2HP	A	1610	-	X	-	-
2	2HP	A	1619	-	X	-	-
2	2HP	A	1620	-	-	-	X
2	2HP	B	1605	-	-	-	X
2	2HP	B	1607	-	X	-	-
2	2HP	B	1608	-	-	-	X
2	2HP	B	1609	-	X	-	-
2	2HP	B	1615	-	X	-	X
2	2HP	B	1616	-	-	-	X
2	2HP	B	1622	-	-	-	X
2	2HP	C	1604	-	X	-	-
2	2HP	C	1611	-	-	-	X
2	2HP	C	1617	-	-	-	X
2	2HP	C	1618	-	X	-	-
3	MPD	A	1702	-	-	-	X
3	MPD	A	1704	X	-	X	X
3	MPD	A	1705	-	-	-	X
3	MPD	A	1706	-	-	-	X
3	MPD	A	1716	-	-	-	X
3	MPD	A	1717	X	-	-	-
3	MPD	A	1720	X	-	X	X
3	MPD	B	1703	-	-	X	X
3	MPD	B	1707	-	-	-	X
3	MPD	B	1709	-	-	X	X
3	MPD	B	1710	-	-	-	X
3	MPD	B	1711	-	-	X	X
3	MPD	B	1718	X	-	-	X
3	MPD	B	1719	X	-	-	-
3	MPD	B	1721	X	-	-	-
3	MPD	B	1722	X	-	-	-
3	MPD	B	1723	-	-	-	X
3	MPD	B	1724	X	-	-	X
3	MPD	C	1701	-	-	-	X
3	MPD	C	1712	-	-	-	X
3	MPD	C	1713	X	-	X	X
3	MPD	C	1714	-	-	-	X
3	MPD	C	1715	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23334 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.

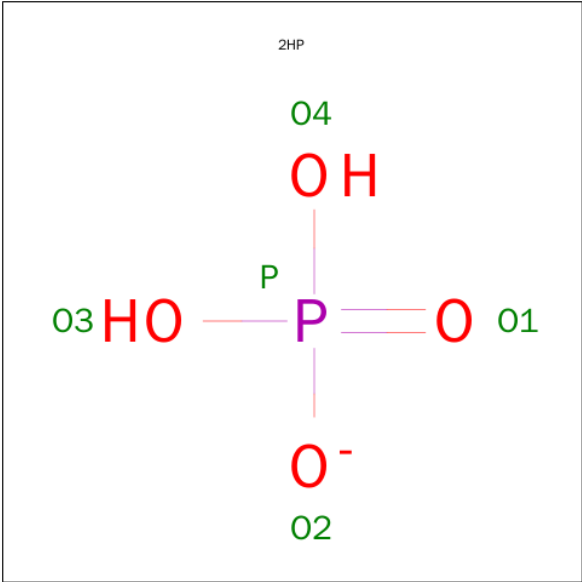
- Molecule 1 is a protein called Hexon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	915	Total	C	N	O	S	2	0	0
			7208	4582	1217	1377	32			
1	B	906	Total	C	N	O	S	2	0	0
			7169	4562	1206	1369	32			
1	C	909	Total	C	N	O	S	2	0	0
			7134	4540	1201	1361	32			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	825	ASN	X	SEE REMARK 999	UNP Q8UY79
A	921	LEU	X	SEE REMARK 999	UNP Q8UY79
B	825	ASN	X	SEE REMARK 999	UNP Q8UY79
B	921	LEU	X	SEE REMARK 999	UNP Q8UY79
C	825	ASN	X	SEE REMARK 999	UNP Q8UY79
C	921	LEU	X	SEE REMARK 999	UNP Q8UY79

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



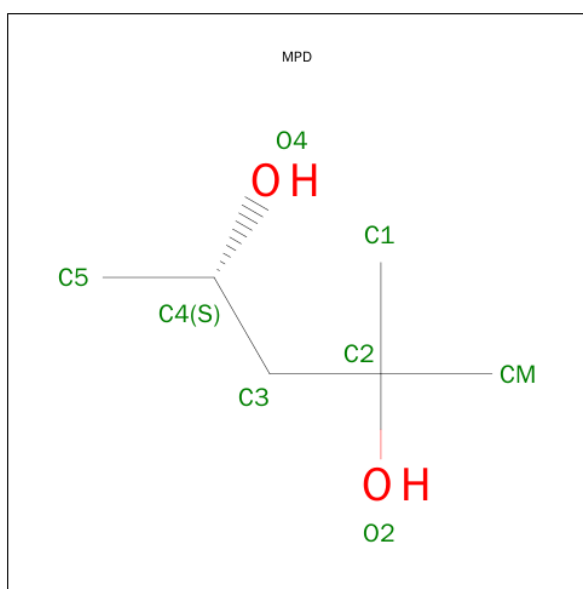
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total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

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

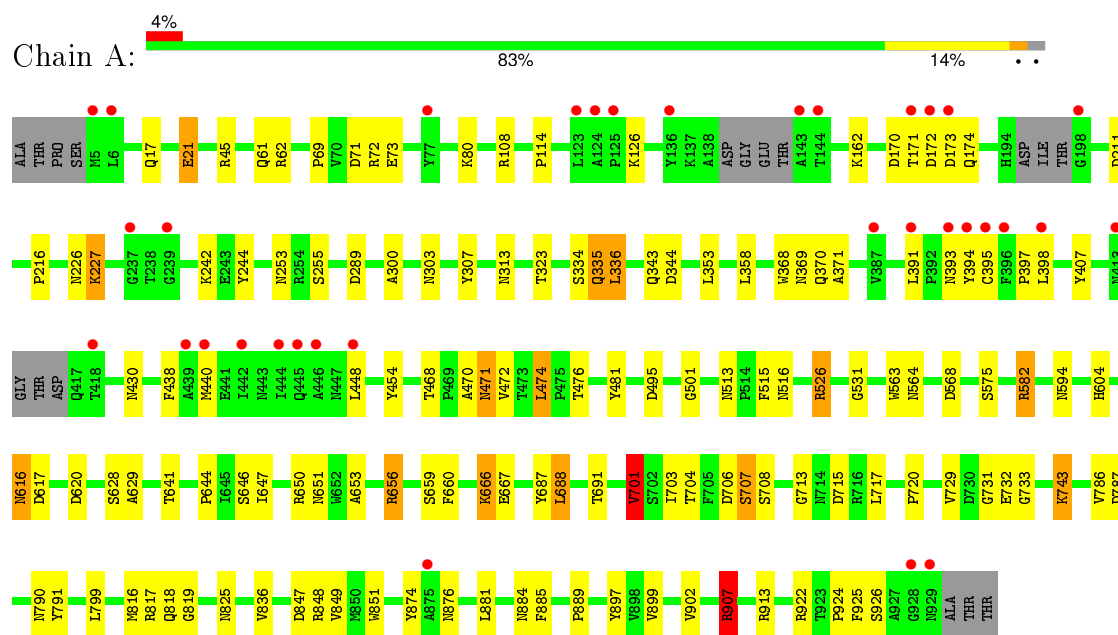
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	542	Total 542	O 542	0	0
4	B	563	Total 563	O 563	0	0
4	C	416	Total 416	O 416	0	0



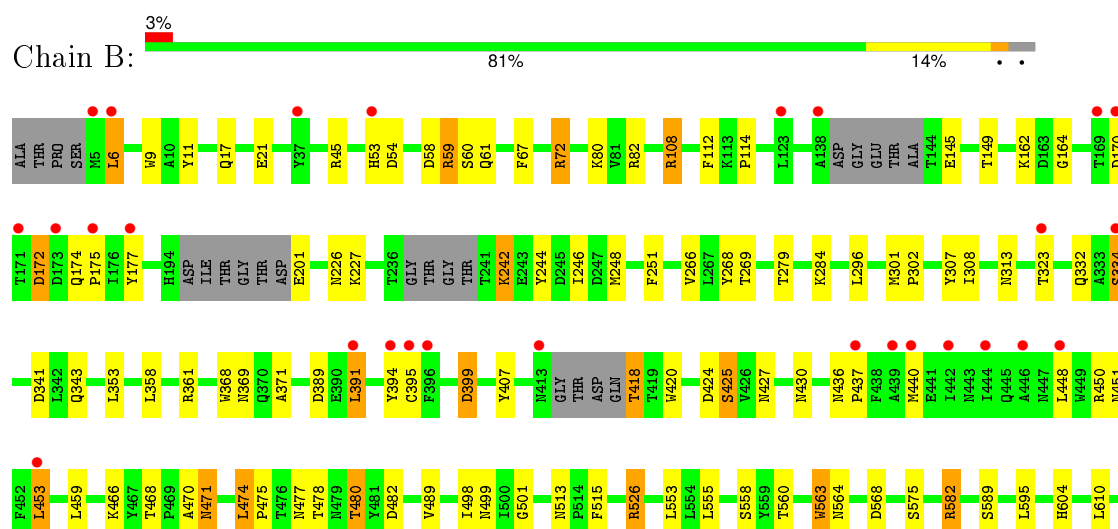
### 3 Residue-property plots

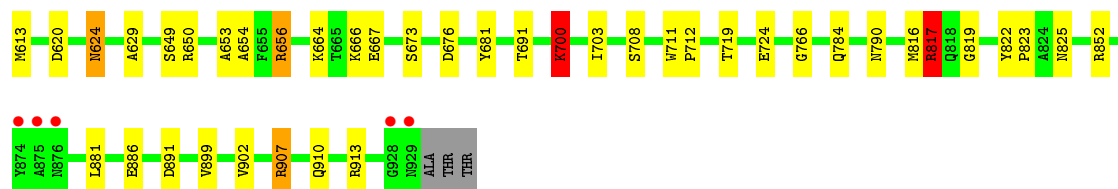
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Hexon

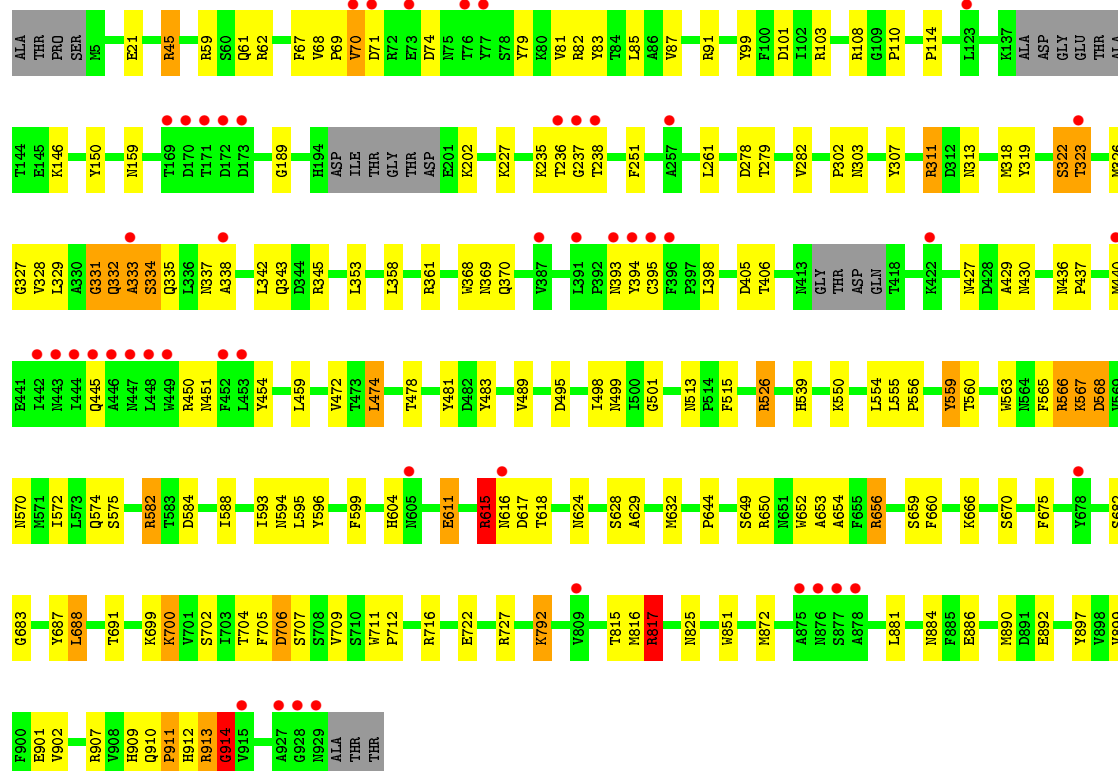
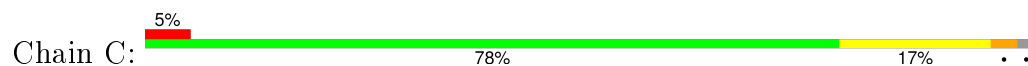


#### • Molecule 1: Hexon





• Molecule 1: Hexon



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.80Å 433.00Å 159.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.10 49.25 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.27-2.10) 93.7 (49.25-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.169 , 0.210 0.168 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 177807 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2HP, MPD

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	0.97	9/7404 (0.1%)	0.95	21/10090 (0.2%)
1	B	1.00	10/7364 (0.1%)	1.04	24/10034 (0.2%)
1	C	1.22	42/7328 (0.6%)	1.02	32/9991 (0.3%)
All	All	1.07	61/22096 (0.3%)	1.00	77/30115 (0.3%)

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
1	A	0	1
1	B	0	1
1	C	0	5
All	All	0	7

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	825	ASN	CG-OD1	-30.50	0.56	1.24
1	B	825	ASN	CG-OD1	-24.34	0.70	1.24
1	C	615	ARG	NE-CZ	22.69	1.62	1.33
1	C	914	GLY	C-O	19.38	1.54	1.23
1	C	328	VAL	C-O	18.29	1.58	1.23

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	ARG	NE-CZ-NH2	-24.16	108.22	120.30
1	B	817	ARG	NE-CZ-NH2	-23.25	108.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	ARG	NE-CZ-NH2	-22.85	108.87	120.30
1	B	817	ARG	NE-CZ-NH1	20.77	130.69	120.30
1	B	656	ARG	NE-CZ-NH2	-19.11	110.74	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	849	VAL	Peptide
1	B	817	ARG	Sidechain
1	C	236	THR	Peptide
1	C	323	THR	Peptide
1	C	331	GLY	Mainchain

## 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	7208	0	6804	109	0
1	B	7169	0	6783	144	0
1	C	7134	0	6705	137	0
2	A	25	0	0	1	0
2	B	60	0	0	2	0
2	C	25	0	0	0	0
3	A	56	0	98	33	0
3	B	96	0	168	53	0
3	C	40	0	70	9	0
4	A	542	0	0	2	0
4	B	563	0	0	10	0
4	C	416	0	0	6	0
All	All	23334	0	20628	385	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 9.

The worst 5 of 385 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:C:913:ARG:CA	1:C:913:ARG:C	1.76	1.49
1:C:567:LYS:NZ	1:C:567:LYS:CE	1.74	1.48
1:B:425:SER:CB	1:B:425:SER:OG	1.65	1.41
1:B:227:LYS:H	3:B:1703:MPD:C1	1.53	1.19
3:B:1711:MPD:H11	3:B:1711:MPD:C5	1.72	1.17

There are no symmetry-related clashes.

## 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	907/932 (97%)	873 (96%)	32 (4%)	2 (0%)	52	53
1	B	896/932 (96%)	858 (96%)	38 (4%)	0	100	100
1	C	901/932 (97%)	858 (95%)	41 (5%)	2 (0%)	52	53
All	All	2704/2796 (97%)	2589 (96%)	111 (4%)	4 (0%)	56	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	SER
1	A	335	GLN
1	C	334	SER
1	C	238	THR

### 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	764/799 (96%)	736 (96%)	28 (4%)	41	41
1	B	764/799 (96%)	730 (96%)	34 (4%)	34	32
1	C	750/799 (94%)	723 (96%)	27 (4%)	42	43
All	All	2278/2397 (95%)	2189 (96%)	89 (4%)	39	39

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	353	LEU
1	B	471	ASN
1	C	670	SER
1	B	358	LEU
1	B	418	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	436	ASN
1	B	624	ASN
1	C	825	ASN
1	B	471	ASN
1	B	790	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 ⓘ

46 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	2HP	A	1602	-	4,4,4	4.31	2 (50%)	6,6,6	1.41	1 (16%)
2	2HP	A	1603	-	4,4,4	4.09	2 (50%)	6,6,6	0.92	0
2	2HP	A	1610	-	4,4,4	4.00	2 (50%)	6,6,6	2.01	2 (33%)
2	2HP	A	1619	-	4,4,4	4.83	2 (50%)	6,6,6	1.39	2 (33%)
2	2HP	A	1620	-	4,4,4	4.46	2 (50%)	6,6,6	0.80	0
3	MPD	A	1702	-	6,7,7	0.44	0	7,10,10	2.27	5 (71%)
3	MPD	A	1704	-	6,7,7	0.75	0	7,10,10	0.86	0
3	MPD	A	1705	-	6,7,7	0.30	0	7,10,10	0.96	1 (14%)
3	MPD	A	1706	-	6,7,7	0.26	0	7,10,10	0.95	1 (14%)
3	MPD	A	1716	-	6,7,7	0.98	0	7,10,10	0.98	0
3	MPD	A	1717	-	6,7,7	0.56	0	7,10,10	0.79	0
3	MPD	A	1720	-	6,7,7	0.37	0	7,10,10	0.48	0
2	2HP	B	1601	-	4,4,4	3.77	2 (50%)	6,6,6	1.15	0
2	2HP	B	1605	-	4,4,4	4.48	2 (50%)	6,6,6	1.61	1 (16%)
2	2HP	B	1606	-	4,4,4	4.07	2 (50%)	6,6,6	1.11	0
2	2HP	B	1607	-	4,4,4	4.20	2 (50%)	6,6,6	1.68	2 (33%)
2	2HP	B	1608	-	4,4,4	4.51	2 (50%)	6,6,6	1.08	0
2	2HP	B	1609	-	4,4,4	3.34	2 (50%)	6,6,6	2.63	5 (83%)
2	2HP	B	1612	-	4,4,4	4.53	2 (50%)	6,6,6	1.22	1 (16%)
2	2HP	B	1614	-	4,4,4	4.32	2 (50%)	6,6,6	1.19	1 (16%)
2	2HP	B	1615	-	4,4,4	4.88	2 (50%)	6,6,6	1.88	3 (50%)
2	2HP	B	1616	-	4,4,4	4.72	2 (50%)	6,6,6	0.81	0
2	2HP	B	1621	-	4,4,4	4.57	2 (50%)	6,6,6	0.59	0
2	2HP	B	1622	-	4,4,4	3.87	2 (50%)	6,6,6	1.96	1 (16%)
3	MPD	B	1703	-	6,7,7	0.69	0	7,10,10	0.65	0
3	MPD	B	1707	-	6,7,7	0.39	0	7,10,10	0.39	0
3	MPD	B	1708	-	6,7,7	0.39	0	7,10,10	0.41	0
3	MPD	B	1709	-	6,7,7	1.12	0	7,10,10	1.19	1 (14%)
3	MPD	B	1710	-	6,7,7	0.42	0	7,10,10	0.72	0
3	MPD	B	1711	-	6,7,7	0.36	0	7,10,10	0.63	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MPD	B	1718	-	6,7,7	0.63	0	7,10,10	1.22	1 (14%)
3	MPD	B	1719	-	6,7,7	0.40	0	7,10,10	0.73	0
3	MPD	B	1721	-	6,7,7	0.30	0	7,10,10	0.56	0
3	MPD	B	1722	-	6,7,7	0.54	0	7,10,10	0.35	0
3	MPD	B	1723	-	6,7,7	0.40	0	7,10,10	0.59	0
3	MPD	B	1724	-	6,7,7	0.33	0	7,10,10	0.61	0
2	2HP	C	1604	-	4,4,4	3.86	2 (50%)	6,6,6	1.85	2 (33%)
2	2HP	C	1611	-	4,4,4	4.52	2 (50%)	6,6,6	0.87	0
2	2HP	C	1613	-	4,4,4	4.40	2 (50%)	6,6,6	1.15	0
2	2HP	C	1617	-	4,4,4	4.75	2 (50%)	6,6,6	1.33	1 (16%)
2	2HP	C	1618	-	4,4,4	4.25	2 (50%)	6,6,6	1.71	2 (33%)
3	MPD	C	1701	-	6,7,7	0.36	0	7,10,10	0.57	0
3	MPD	C	1712	-	6,7,7	0.57	0	7,10,10	0.82	0
3	MPD	C	1713	-	6,7,7	0.56	0	7,10,10	1.07	0
3	MPD	C	1714	-	6,7,7	0.41	0	7,10,10	0.34	0
3	MPD	C	1715	-	6,7,7	0.24	0	7,10,10	0.75	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
2	2HP	A	1602	-	-	0/0/0/0	0/0/0/0
2	2HP	A	1603	-	-	0/0/0/0	0/0/0/0
2	2HP	A	1610	-	-	0/0/0/0	0/0/0/0
2	2HP	A	1619	-	-	0/0/0/0	0/0/0/0
2	2HP	A	1620	-	-	0/0/0/0	0/0/0/0
3	MPD	A	1702	-	-	0/5/5/5	0/0/0/0
3	MPD	A	1704	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	A	1705	-	-	0/5/5/5	0/0/0/0
3	MPD	A	1706	-	-	0/5/5/5	0/0/0/0
3	MPD	A	1716	-	-	0/5/5/5	0/0/0/0
3	MPD	A	1717	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	A	1720	-	1/1/2/2	0/5/5/5	0/0/0/0
2	2HP	B	1601	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1605	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1606	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1607	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1608	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1609	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2HP	B	1612	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1614	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1615	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1616	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1621	-	-	0/0/0/0	0/0/0/0
2	2HP	B	1622	-	-	0/0/0/0	0/0/0/0
3	MPD	B	1703	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1707	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1708	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1709	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1710	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1711	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1718	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	B	1719	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	B	1721	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	B	1722	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	B	1723	-	-	0/5/5/5	0/0/0/0
3	MPD	B	1724	-	1/1/2/2	0/5/5/5	0/0/0/0
2	2HP	C	1604	-	-	0/0/0/0	0/0/0/0
2	2HP	C	1611	-	-	0/0/0/0	0/0/0/0
2	2HP	C	1613	-	-	0/0/0/0	0/0/0/0
2	2HP	C	1617	-	-	0/0/0/0	0/0/0/0
2	2HP	C	1618	-	-	0/0/0/0	0/0/0/0
3	MPD	C	1701	-	-	0/5/5/5	0/0/0/0
3	MPD	C	1712	-	-	0/5/5/5	0/0/0/0
3	MPD	C	1713	-	1/1/2/2	0/5/5/5	0/0/0/0
3	MPD	C	1714	-	-	0/5/5/5	0/0/0/0
3	MPD	C	1715	-	-	0/5/5/5	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1609	2HP	P-O4	4.66	1.73	1.55
2	B	1601	2HP	P-O4	4.76	1.73	1.55
2	B	1609	2HP	P-O3	4.79	1.73	1.55
2	B	1622	2HP	P-O4	4.86	1.74	1.55
2	C	1604	2HP	P-O4	5.35	1.76	1.55

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1609	2HP	O4-P-O2	-4.19	97.38	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1702	MPD	C2-C3-C4	-3.97	97.87	116.66
2	C	1604	2HP	O3-P-O2	-3.26	99.97	109.06
2	B	1615	2HP	O3-P-O2	-2.77	101.34	109.06
2	B	1609	2HP	O3-P-O1	-2.75	101.18	109.06

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1720	MPD	C4
3	C	1713	MPD	C4
3	B	1718	MPD	C4
3	B	1724	MPD	C4
3	A	1717	MPD	C4

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1610	2HP	1	0
3	A	1702	MPD	1	0
3	A	1704	MPD	10	0
3	A	1705	MPD	2	0
3	A	1716	MPD	5	0
3	A	1717	MPD	4	0
3	A	1720	MPD	11	0
2	B	1606	2HP	1	0
2	B	1616	2HP	1	0
3	B	1703	MPD	13	0
3	B	1707	MPD	4	0
3	B	1709	MPD	13	0
3	B	1711	MPD	7	0
3	B	1718	MPD	4	0
3	B	1719	MPD	3	0
3	B	1721	MPD	1	0
3	B	1722	MPD	3	0
3	B	1723	MPD	5	0
3	C	1713	MPD	8	0
3	C	1714	MPD	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	915/932 (98%)	0.02	34 (3%)	45	54	29, 36, 52, 73	1 (0%)
1	B	906/932 (97%)	0.08	32 (3%)	48	57	28, 36, 49, 73	1 (0%)
1	C	909/932 (97%)	0.24	48 (5%)	30	39	28, 36, 50, 73	1 (0%)
All	All	2730/2796 (97%)	0.11	114 (4%)	40	49	28, 36, 50, 73	3 (0%)

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	928	GLY	9.2
1	C	876	ASN	8.6
1	A	5	MET	6.8
1	C	875	ALA	6.5
1	C	395	CYS	6.2

### 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( $\text{\AA}^2$ )	Q<0.9
2	2HP	A	1603	5/5	0.98	0.22	12.78	42,43,44,45	0
2	2HP	A	1620	5/5	0.94	0.36	11.93	69,71,71,71	0
3	MPD	C	1712	8/8	0.87	0.23	11.79	42,45,46,49	0
2	2HP	B	1615	5/5	0.96	0.25	10.99	41,41,42,42	0
3	MPD	C	1714	8/8	0.91	0.26	8.85	54,55,56,57	0
2	2HP	B	1608	5/5	0.89	0.30	8.34	78,78,79,79	0
3	MPD	A	1706	8/8	0.93	0.20	8.29	60,61,62,63	0
2	2HP	C	1617	5/5	0.91	0.28	7.05	46,50,52,53	0
3	MPD	C	1701	8/8	0.84	0.22	6.20	55,55,57,57	0
3	MPD	A	1720	8/8	0.82	0.25	6.15	63,65,66,66	0
3	MPD	B	1710	8/8	0.95	0.21	5.44	44,45,47,47	0
3	MPD	A	1716	8/8	0.82	0.21	5.26	33,36,41,44	0
2	2HP	B	1622	5/5	0.86	0.22	5.08	34,37,46,46	0
3	MPD	B	1718	8/8	0.81	0.25	4.88	34,37,44,44	0
2	2HP	B	1616	5/5	0.97	0.29	4.50	58,59,61,61	0
3	MPD	A	1705	8/8	0.94	0.19	4.44	58,58,58,59	0
3	MPD	C	1715	8/8	0.94	0.25	4.13	64,66,67,67	0
3	MPD	C	1713	8/8	0.90	0.19	4.09	39,42,44,44	0
3	MPD	B	1724	8/8	0.95	0.16	3.31	58,60,61,61	0
3	MPD	A	1704	8/8	0.84	0.22	3.29	35,39,41,46	0
2	2HP	B	1605	5/5	0.92	0.18	3.28	53,55,56,56	0
3	MPD	B	1711	8/8	0.93	0.20	3.27	55,55,56,57	0
2	2HP	C	1611	5/5	0.96	0.22	3.21	54,54,55,56	0
3	MPD	A	1702	8/8	0.90	0.14	2.57	41,45,46,48	0
3	MPD	B	1703	8/8	0.73	0.22	2.49	61,62,63,64	0
3	MPD	B	1707	8/8	0.91	0.21	2.26	49,52,54,54	0
3	MPD	B	1723	8/8	0.86	0.20	2.20	70,74,75,76	0
3	MPD	B	1709	8/8	0.84	0.15	2.02	28,33,39,42	0
2	2HP	C	1604	5/5	0.97	0.14	1.90	51,52,53,53	0
2	2HP	C	1613	5/5	0.95	0.16	1.27	49,51,52,52	0
2	2HP	B	1609	5/5	0.98	0.13	1.21	35,35,37,38	0
3	MPD	B	1708	8/8	0.85	0.20	0.95	71,72,72,73	0
2	2HP	B	1621	5/5	0.93	0.27	0.72	72,72,73,74	0
2	2HP	B	1606	5/5	0.95	0.16	0.60	52,52,55,56	0
2	2HP	A	1602	5/5	0.99	0.17	0.58	36,39,43,45	0
2	2HP	A	1610	5/5	0.97	0.15	0.50	51,51,53,54	0
3	MPD	B	1719	8/8	0.93	0.11	0.12	44,47,49,49	0
2	2HP	B	1607	5/5	0.96	0.11	-0.61	45,45,48,48	0
2	2HP	C	1618	5/5	0.96	0.11	-1.36	56,57,58,59	0
2	2HP	B	1601	5/5	0.98	0.07	-2.82	37,38,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	A	1717	8/8	0.44	0.24	-	67,69,70,70	0
2	2HP	B	1612	5/5	0.84	0.23	-	77,78,79,79	0
3	MPD	B	1721	8/8	0.89	0.24	-	61,62,63,64	0
2	2HP	A	1619	5/5	0.92	0.25	-	59,60,60,61	0
3	MPD	B	1722	8/8	0.59	0.17	-	95,95,95,95	0
2	2HP	B	1614	5/5	0.97	0.16	-	60,60,61,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.