



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:05 pm GMT

PDB ID : 2C1J  
Title : Molecular basis for the recognition of phosphorylated and phosphoacetylated histone H3 by 14-3-3  
Authors : Welburn, J.P.I.; Macdonald, N.; Noble, M.E.M.; Nguyen, A.; Yaffe, M.B.; Clynes, D.; Moggs, J.G.; Orphanides, G.; Thomson, S.; Edmunds, J.W.; Clayton, A.L.; Endicott, J.A.; Mahadevan, L.C.  
Deposited on : 2005-09-15  
Resolution : 2.60 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

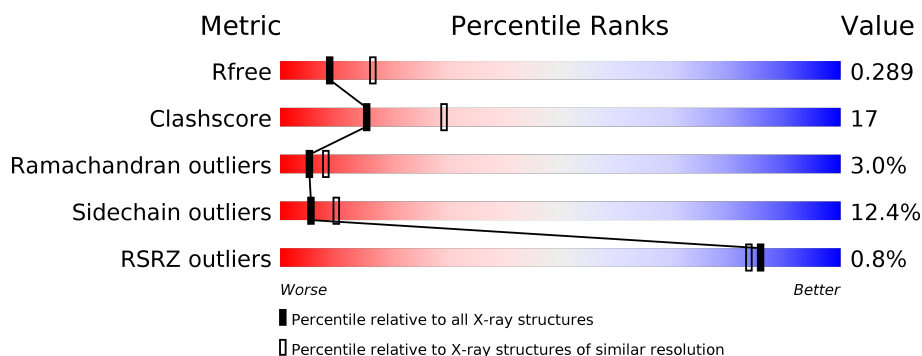
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	258	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 62%, green 23%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>62%</span> <span>23%</span> <span>•</span> <span>11%</span> </div> </div>
1	B	258	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 58%, yellow 28%, orange 1%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>58%</span> <span>28%</span> <span>•</span> <span>11%</span> </div> </div>
2	C	8	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 25%, yellow 38%, orange 25%, red 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>25%</span> <span>38%</span> <span>25%</span> <span>13%</span> </div> </div>
2	D	8	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 13%, yellow 38%, orange 25%, red 25%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>13%</span> <span>38%</span> <span>25%</span> <span>25%</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SEP	C	10	-	-	X	-
2	ALY	C	9	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3892 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 14-3-3 PROTEIN ZETA/DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1841	1154	309	368	10			
1	B	230	Total	C	N	O	S	0	0	0
			1841	1154	309	368	10			

- Molecule 2 is a protein called HISTONE H3 ACETYLPHOSPHOPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			62	34	13	14	1			
2	D	8	Total	C	N	O	P	0	0	0
			62	34	13	14	1			

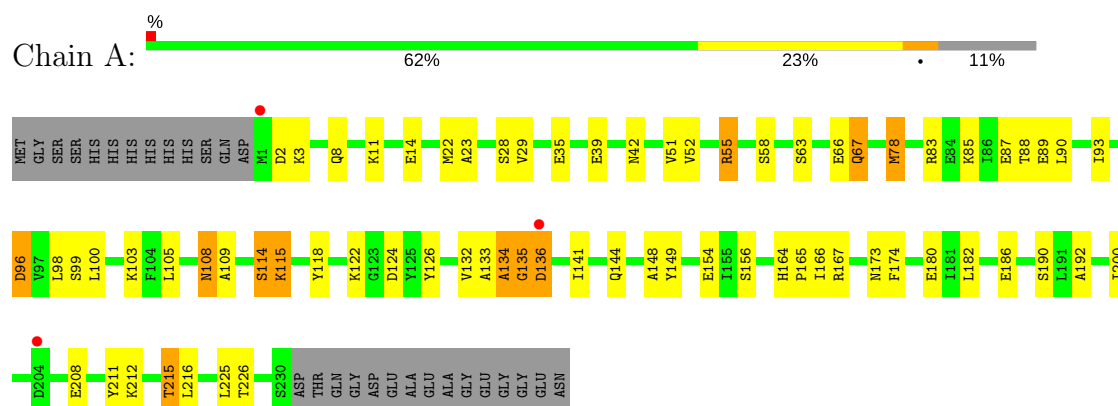
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	27	Total	O	0	0
			27	27		
3	C	3	Total	O	0	0
			3	3		
3	D	5	Total	O	0	0
			5	5		

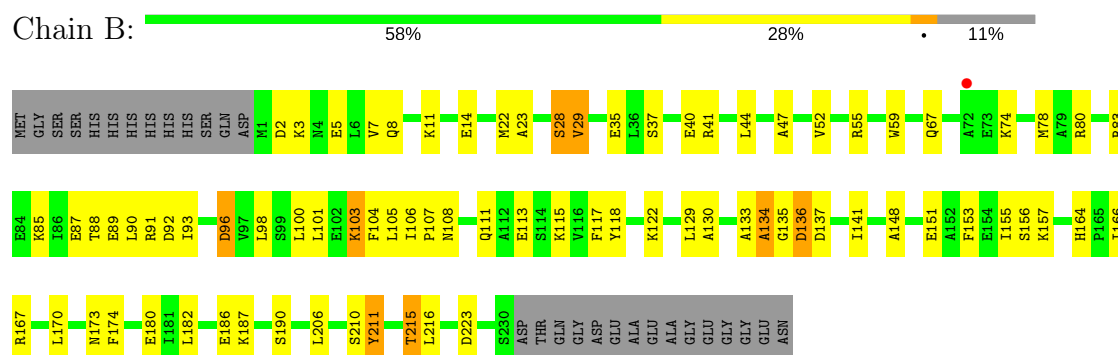
### 3 Residue-property plots [i](#)

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

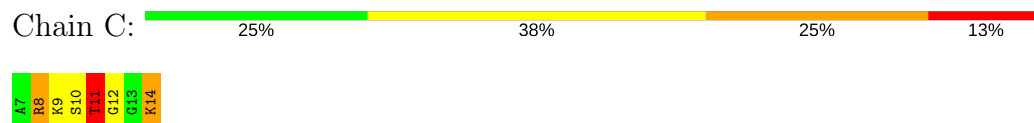
#### • Molecule 1: 14-3-3 PROTEIN ZETA/DELTA



#### • Molecule 1: 14-3-3 PROTEIN ZETA/DELTA



#### • Molecule 2: HISTONE H3 ACETYLPHOSPHOPEPTIDE



#### • Molecule 2: HISTONE H3 ACETYLPHOSPHOPEPTIDE



A7	R8	K9	S10	T11	G12	G13	K14
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.19Å 72.41Å 71.16Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	69.34 – 2.60 21.20 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.34-2.60) 99.9 (21.20-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.227 , 0.292 0.227 , 0.289	Depositor DCC
$R_{free}$ test set	1113 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , -4.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.459 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% 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, 0.333 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: ALY, SEP

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	0.65	0/1866	0.73	0/2509
1	B	0.64	0/1866	0.74	0/2509
2	C	0.96	0/38	1.34	0/46
2	D	0.83	0/38	1.52	1/46 (2.2%)
All	All	0.65	0/3808	0.76	1/5110 (0.0%)

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	D	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	14	LYS	N-CA-C	5.09	124.74	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	13	GLY	Peptide
2	D	8	ARG	Mainchain
2	D	9	ALY	Mainchain



## 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	1841	0	1830	52	0
1	B	1841	0	1830	56	0
2	C	62	0	63	18	0
2	D	62	0	59	7	0
3	A	51	0	0	7	0
3	B	27	0	0	5	0
3	C	3	0	0	0	0
3	D	5	0	0	2	0
All	All	3892	0	3782	124	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 17.

All (124) 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)
2:C:9:ALY:C	2:C:10:SEP:H2	1.46	1.19
1:A:42:ASN:HB3	3:A:2010:HOH:O	1.45	1.12
1:A:133:ALA:HA	1:A:134:ALA:HB2	1.48	0.96
1:B:164:HIS:HD2	1:B:166:ILE:H	1.14	0.95
1:B:210:SER:HB3	3:B:2026:HOH:O	1.64	0.95
1:B:80:ARG:HD3	3:B:2012:HOH:O	1.65	0.95
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.31	0.94
2:C:8:ARG:C	2:C:9:ALY:H2	1.62	0.93
1:A:180:GLU:OE1	2:C:8:ARG:HD3	1.69	0.93
2:C:8:ARG:O	2:C:9:ALY:N	2.08	0.87
1:A:164:HIS:HD2	1:A:166:ILE:H	1.22	0.87
1:B:156:SER:HB2	1:B:167:ARG:HG3	1.58	0.85
1:B:133:ALA:HA	1:B:134:ALA:HB2	1.61	0.83
1:B:8:GLN:HB3	3:B:2002:HOH:O	1.79	0.83
1:A:156:SER:HB2	1:A:167:ARG:HG3	1.60	0.82
1:A:180:GLU:OE1	2:C:8:ARG:CD	2.28	0.81
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.44	0.81
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.16	0.80
1:A:83:ARG:HG2	1:A:83:ARG:NH1	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ALY:CA	2:C:10:SEP:H2	1.96	0.78
2:C:9:ALY:CA	2:C:10:SEP:N	2.46	0.77
1:B:173:ASN:HD21	2:D:11:THR:HB	1.50	0.77
1:B:164:HIS:CD2	1:B:166:ILE:H	2.01	0.76
1:A:66:GLU:OE2	1:A:83:ARG:NE	2.20	0.74
1:A:85:LYS:HE2	3:A:2021:HOH:O	1.88	0.73
1:B:135:GLY:O	1:B:136:ASP:HB2	1.88	0.72
2:C:9:ALY:C	2:C:10:SEP:CA	2.68	0.71
1:A:133:ALA:CA	1:A:134:ALA:HB2	2.23	0.68
1:A:8:GLN:HG3	3:A:2003:HOH:O	1.93	0.67
1:A:173:ASN:HD21	2:C:11:THR:HB	1.61	0.66
1:B:103:LYS:HB2	1:B:104:PHE:CD1	2.31	0.65
1:B:180:GLU:OE1	2:D:8:ARG:HD3	1.98	0.64
1:B:153:PHE:HA	1:B:170:LEU:HD21	1.80	0.63
2:C:9:ALY:O	2:C:10:SEP:N	2.29	0.63
1:A:164:HIS:CD2	1:A:166:ILE:H	2.11	0.63
1:B:59:TRP:HE1	1:B:87:GLU:HG3	1.63	0.62
1:A:135:GLY:O	1:A:136:ASP:HB2	2.00	0.62
1:B:164:HIS:HD2	1:B:166:ILE:N	1.92	0.61
2:C:8:ARG:CA	2:C:9:ALY:N	2.64	0.60
1:A:11:LYS:HE2	1:A:39:GLU:OE2	2.02	0.60
1:B:7:VAL:O	1:B:11:LYS:HG3	2.00	0.60
1:B:3:LYS:HD3	1:B:40:GLU:OE2	2.02	0.60
1:B:133:ALA:CA	1:B:134:ALA:HB2	2.31	0.60
1:A:109:ALA:HB3	1:A:115:LYS:HD2	1.84	0.59
1:A:99:SER:HB2	3:A:2026:HOH:O	2.01	0.59
2:C:8:ARG:C	2:C:9:ALY:H	1.99	0.59
2:D:7:ALA:N	3:D:2002:HOH:O	2.35	0.59
1:A:78:MET:HE2	1:A:78:MET:HA	1.83	0.58
1:B:28:SER:O	1:B:29:VAL:C	2.42	0.58
1:A:98:LEU:HD22	1:A:126:TYR:CE2	2.39	0.57
1:B:157:LYS:HB2	3:B:2019:HOH:O	2.04	0.57
1:A:55:ARG:HD3	1:A:93:ILE:HD13	1.85	0.57
1:A:133:ALA:HB1	1:A:134:ALA:HB3	1.86	0.57
2:C:9:ALY:HCA	2:C:10:SEP:N	2.20	0.57
1:A:156:SER:CB	1:A:167:ARG:HG3	2.33	0.56
1:B:59:TRP:NE1	1:B:87:GLU:HG3	2.20	0.56
1:B:153:PHE:CZ	1:B:157:LYS:HE3	2.40	0.56
1:A:133:ALA:CA	1:A:134:ALA:CB	2.82	0.56
1:A:109:ALA:HB1	1:A:114:SER:HB3	1.87	0.55
1:A:103:LYS:HE2	3:A:2030:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:O	1:A:89:GLU:C	2.45	0.55
1:B:37:SER:OG	1:B:40:GLU:HG3	2.08	0.53
1:B:122:LYS:HD3	1:B:148:ALA:HB2	1.91	0.52
1:A:108:ASN:N	1:A:108:ASN:HD22	2.09	0.51
1:A:124:ASP:HA	1:A:149:TYR:OH	2.10	0.51
1:B:55:ARG:HD2	1:B:93:ILE:HD13	1.92	0.51
1:B:105:LEU:HD22	1:B:118:TYR:CZ	2.46	0.51
1:B:211:TYR:O	1:B:215:THR:HB	2.11	0.51
1:A:14:GLU:HB2	1:A:22:MET:CE	2.41	0.51
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.19	0.50
1:A:180:GLU:OE1	2:C:8:ARG:HD2	2.11	0.50
1:B:106:ILE:HB	1:B:107:PRO:HD3	1.95	0.49
1:A:211:TYR:O	1:A:215:THR:HB	2.12	0.49
1:A:109:ALA:CB	1:A:114:SER:HB3	2.43	0.49
2:D:9:ALY:HCA	3:D:2004:HOH:O	2.13	0.49
1:A:122:LYS:HG2	1:A:148:ALA:HB2	1.95	0.48
1:B:41:ARG:NH1	1:B:113:GLU:OE2	2.42	0.48
1:A:135:GLY:O	1:A:136:ASP:CB	2.61	0.48
1:B:133:ALA:HA	1:B:134:ALA:CB	2.40	0.48
2:C:8:ARG:NH2	2:C:10:SEP:O1P	2.44	0.48
1:B:59:TRP:HE1	1:B:87:GLU:CG	2.27	0.47
2:C:9:ALY:HCA	2:C:10:SEP:H2	1.78	0.47
1:A:67:GLN:N	1:A:67:GLN:HE21	2.12	0.47
1:B:156:SER:CB	1:B:167:ARG:HG3	2.37	0.47
1:A:164:HIS:HD2	1:A:166:ILE:N	2.02	0.46
1:B:223:ASP:HB3	2:D:9:ALY:HH31	1.97	0.46
1:B:206:LEU:HD22	1:B:211:TYR:HA	1.97	0.46
1:B:151:GLU:O	1:B:155:ILE:HG13	2.15	0.46
1:B:22:MET:HG2	1:B:47:ALA:HB2	1.97	0.46
1:A:164:HIS:CD2	1:A:165:PRO:CD	2.93	0.46
1:B:91:ARG:HG2	1:B:129:LEU:CD2	2.45	0.45
2:C:11:THR:HG22	2:C:12:GLY:N	2.31	0.45
1:A:51:VAL:HG13	1:A:55:ARG:NH1	2.31	0.45
1:B:153:PHE:CA	1:B:170:LEU:HD21	2.46	0.45
1:B:23:ALA:HA	1:B:47:ALA:HB1	1.98	0.45
2:D:10:SEP:O	2:D:13:GLY:N	2.40	0.45
1:B:133:ALA:CA	1:B:134:ALA:CB	2.94	0.45
1:A:78:MET:CE	1:A:78:MET:HA	2.46	0.44
1:A:133:ALA:HB1	1:A:134:ALA:CB	2.47	0.44
1:B:173:ASN:ND2	2:D:11:THR:HB	2.25	0.43
1:B:135:GLY:O	1:B:136:ASP:CB	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HD3	1:A:93:ILE:CD1	2.48	0.43
1:B:14:GLU:HB2	1:B:22:MET:SD	2.58	0.43
1:B:41:ARG:HD3	1:B:117:PHE:CD1	2.53	0.43
1:B:88:THR:O	1:B:89:GLU:C	2.57	0.43
1:A:154:GLU:CB	3:A:2036:HOH:O	2.67	0.43
1:A:78:MET:HE1	1:B:5:GLU:OE2	2.19	0.42
1:A:51:VAL:HG13	1:A:55:ARG:HH11	1.85	0.42
1:A:154:GLU:HB3	3:A:2036:HOH:O	2.20	0.41
1:A:192:ALA:HB3	1:A:225:LEU:HD21	2.02	0.41
1:A:28:SER:O	1:A:29:VAL:C	2.58	0.41
1:A:63:SER:O	1:A:67:GLN:NE2	2.54	0.41
1:B:157:LYS:HA	1:B:167:ARG:NH1	2.35	0.41
1:B:83:ARG:NH1	1:B:83:ARG:CG	2.84	0.41
1:B:35:GLU:HG3	1:B:108:ASN:HB3	2.03	0.41
1:B:186:GLU:HG3	1:B:187:LYS:H	1.84	0.41
2:C:14:LYS:H	2:C:14:LYS:HD3	1.85	0.41
1:B:98:LEU:HA	1:B:101:LEU:HD12	2.02	0.41
1:B:186:GLU:HG3	1:B:187:LYS:N	2.36	0.41
1:B:130:ALA:HA	1:B:141:ILE:HD11	2.03	0.40
1:B:59:TRP:CD1	1:B:87:GLU:HG3	2.56	0.40
1:A:105:LEU:HD22	1:A:118:TYR:CZ	2.56	0.40
1:B:85:LYS:HE3	3:B:2013:HOH:O	2.22	0.40
1:A:87:GLU:HG3	1:A:132:VAL:HG13	2.04	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	228/258 (88%)	208 (91%)	14 (6%)	6 (3%)	6	10
1	B	228/258 (88%)	207 (91%)	16 (7%)	5 (2%)	8	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	4/8 (50%)	2 (50%)	1 (25%)	1 (25%)	0	0
2	D	4/8 (50%)	2 (50%)	0	2 (50%)	0	0
All	All	464/532 (87%)	419 (90%)	31 (7%)	14 (3%)	5	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ALA
1	B	134	ALA
1	B	29	VAL
1	B	96	ASP
1	A	96	ASP
2	D	8	ARG
2	C	11	THR
2	D	11	THR
1	A	23	ALA
1	A	58	SER
1	B	136	ASP
1	A	136	ASP
1	B	28	SER
1	A	135	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/221 (90%)	174 (87%)	25 (13%)	5	9
1	B	199/221 (90%)	179 (90%)	20 (10%)	9	16
2	C	3/3 (100%)	0	3 (100%)	0	0
2	D	3/3 (100%)	1 (33%)	2 (67%)	0	0
All	All	404/448 (90%)	354 (88%)	50 (12%)	5	10

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	LYS
1	A	35	GLU
1	A	52	VAL
1	A	55	ARG
1	A	67	GLN
1	A	78	MET
1	A	90	LEU
1	A	96	ASP
1	A	100	LEU
1	A	108	ASN
1	A	114	SER
1	A	115	LYS
1	A	141	ILE
1	A	144	GLN
1	A	174	PHE
1	A	182	LEU
1	A	186	GLU
1	A	190	SER
1	A	200	ILE
1	A	208	GLU
1	A	212	LYS
1	A	215	THR
1	A	216	LEU
1	A	226	THR
1	B	2	ASP
1	B	44	LEU
1	B	52	VAL
1	B	67	GLN
1	B	74	LYS
1	B	78	MET
1	B	90	LEU
1	B	92	ASP
1	B	96	ASP
1	B	100	LEU
1	B	103	LYS
1	B	111	GLN
1	B	115	LYS
1	B	137	ASP
1	B	174	PHE
1	B	182	LEU
1	B	190	SER
1	B	211	TYR

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Mol	Chain	Res	Type
1	B	215	THR
1	B	216	LEU
2	C	8	ARG
2	C	11	THR
2	C	14	LYS
2	D	8	ARG
2	D	11	THR

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

Mol	Chain	Res	Type
1	A	67	GLN
1	A	108	ASN
1	A	164	HIS
1	B	76	GLN
1	B	108	ASN
1	B	164	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	SEP	C	10	2	9,9,10	1.35	1 (11%)	9,12,14	1.34	1 (11%)
2	ALY	C	9	2	11,11,12	0.69	0	9,12,14	1.57	2 (22%)
2	SEP	D	10	2	9,9,10	1.19	1 (11%)	9,12,14	1.65	2 (22%)
2	ALY	D	9	2	11,11,12	0.55	0	9,12,14	1.89	3 (33%)

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	SEP	C	10	2	-	0/5/8/10	0/0/0/0
2	ALY	C	9	2	-	0/8/10/12	0/0/0/0
2	SEP	D	10	2	-	0/5/8/10	0/0/0/0
2	ALY	D	9	2	-	0/8/10/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	SEP	P-O1P	2.74	1.60	1.50
2	C	10	SEP	P-O1P	3.25	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	ALY	CB-CA-C	-2.75	107.11	111.65
2	D	10	SEP	P-OG-CB	-2.71	110.83	118.30
2	D	10	SEP	O3P-P-O1P	-2.46	100.87	110.50
2	D	9	ALY	O-C-CA	-2.13	119.13	125.02
2	C	10	SEP	O2P-P-OG	2.38	113.07	106.73
2	C	9	ALY	CB-CA-C	2.57	115.89	111.65
2	C	9	ALY	CE-NZ-CH	2.70	126.84	122.49
2	D	9	ALY	CE-NZ-CH	3.78	128.59	122.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	10	SEP	8	0
2	C	9	ALY	11	0
2	D	10	SEP	1	0
2	D	9	ALY	2	0



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	230/258 (89%)	-0.20	3 (1%) 77 73	2, 9, 24, 35	0
1	B	230/258 (89%)	-0.21	1 (0%) 92 91	2, 9, 24, 35	0
2	C	6/8 (75%)	-0.14	0 100 100	8, 11, 15, 18	0
2	D	6/8 (75%)	-0.31	0 100 100	8, 11, 15, 17	0
All	All	472/532 (88%)	-0.20	4 (0%) 86 83	2, 9, 24, 35	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.1
1	A	204	ASP	2.7
1	A	136	ASP	2.5
1	B	72	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	D	10	10/11	0.98	0.13	-	2,7,9,9	0
2	ALY	D	9	12/13	0.96	0.14	-	8,11,21,24	0
2	ALY	C	9	12/13	0.97	0.21	-	8,11,20,22	0
2	SEP	C	10	10/11	0.98	0.16	-	3,8,9,9	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.