



# Full wwPDB X-ray Structure Validation Report i

Nov 14, 2023 – 06:39 PM JST

PDB ID : 6A0X  
Title : Crystal structure of broadly neutralizing antibody 13D4  
Authors : Li, S.; Li, T.  
Deposited on : 2018-06-06  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

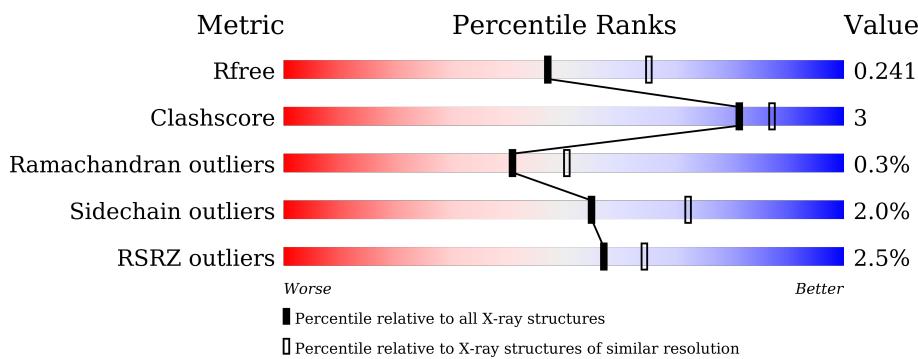
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.



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Mol	Chain	Length	Quality of chain			
2	F	214	4%	94%	5%	.
2	H	214	5%	95%	..	

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
1	PCA	A	1	-	-	-	X

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13751 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 Antibody 13D4, Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1681	1065	276	333	7			
1	C	224	Total	C	N	O	S	0	0	0
			1681	1065	276	333	7			
1	E	224	Total	C	N	O	S	0	0	0
			1681	1065	276	333	7			
1	G	224	Total	C	N	O	S	0	0	0
			1681	1065	276	333	7			

- Molecule 2 is a protein called Antibody 13D4, Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1659	1031	283	337	8			
2	D	214	Total	C	N	O	S	0	0	0
			1659	1031	283	337	8			
2	F	214	Total	C	N	O	S	0	0	0
			1659	1031	283	337	8			
2	H	214	Total	C	N	O	S	0	0	0
			1659	1031	283	337	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	80	Total	O	0	0
			80	80		
3	C	40	Total	O	0	0
			40	40		
3	D	70	Total	O	0	0
			70	70		

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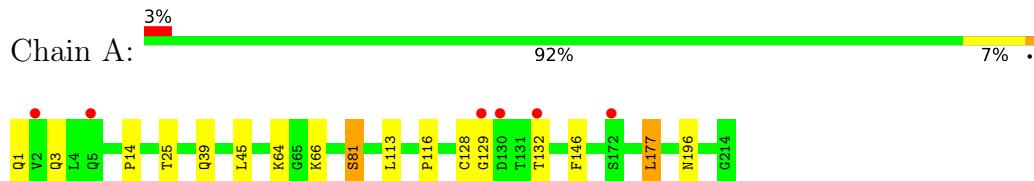
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	49	Total O 49 49	0	0
3	F	35	Total O 35 35	0	0
3	G	53	Total O 53 53	0	0
3	H	27	Total O 27 27	0	0

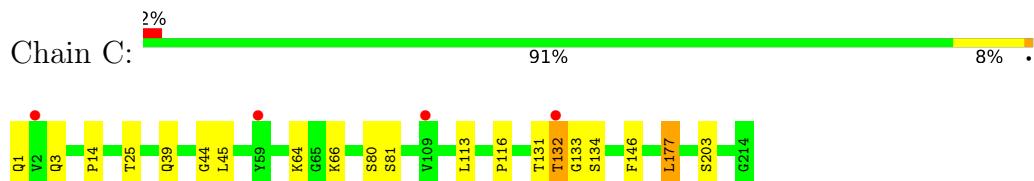
### 3 Residue-property plots [\(i\)](#)

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

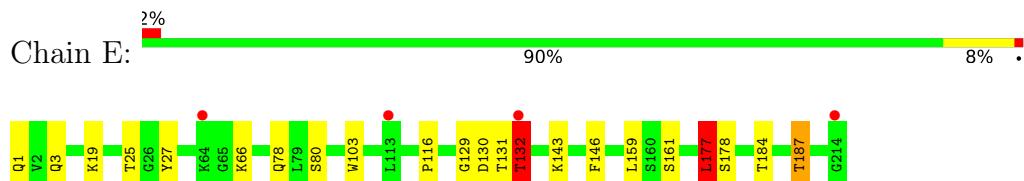
- Molecule 1: Antibody 13D4, Fab Heavy Chain



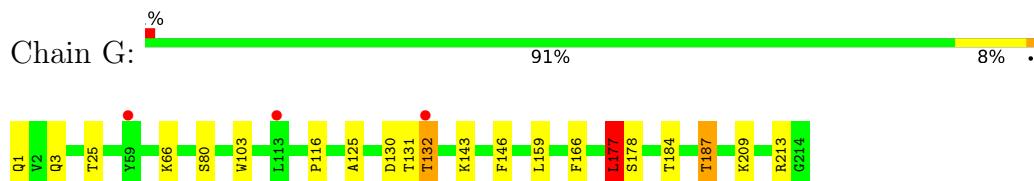
- Molecule 1: Antibody 13D4, Fab Heavy Chain



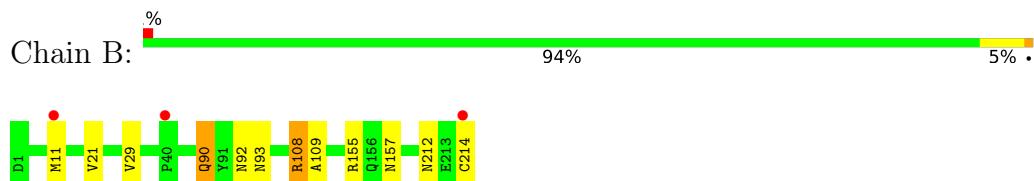
- Molecule 1: Antibody 13D4, Fab Heavy Chain



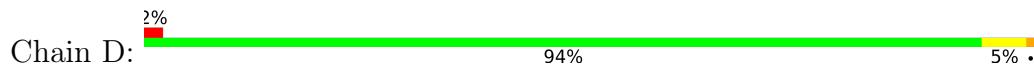
- Molecule 1: Antibody 13D4, Fab Heavy Chain



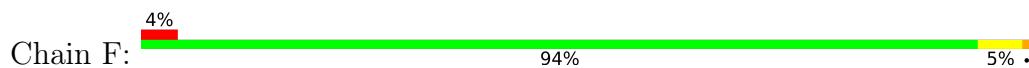
- Molecule 2: Antibody 13D4, Fab Light Chain



- Molecule 2: Antibody 13D4, Fab Light Chain



- Molecule 2: Antibody 13D4, Fab Light Chain



- Molecule 2: Antibody 13D4, Fab Light Chain



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.38Å 108.96Å 108.18Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	48.66 – 2.30 48.66 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.66-2.30) 99.2 (48.66-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.61 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
$R$ , $R_{free}$	0.205 , 0.243 0.209 , 0.241	Depositor DCC
$R_{free}$ test set	4063 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.6	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50$ , $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k 0.006 for -h,l,k 0.458 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.42% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PCA

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	0.25	0/1720	0.50	1/2354 (0.0%)
1	C	0.25	0/1720	0.49	1/2354 (0.0%)
1	E	0.25	0/1720	0.53	1/2354 (0.0%)
1	G	0.27	0/1720	0.50	1/2354 (0.0%)
2	B	0.26	0/1696	0.48	0/2301
2	D	0.26	0/1696	0.48	0/2301
2	F	0.26	0/1696	0.46	0/2301
2	H	0.26	0/1696	0.46	0/2301
All	All	0.26	0/13664	0.49	4/18620 (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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	LEU	CA-CB-CG	5.43	127.80	115.30
1	C	177	LEU	CA-CB-CG	5.43	127.79	115.30
1	G	177	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	177	LEU	CA-CB-CG	5.31	127.52	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	212	ASN	Peptide

## 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	1681	0	1622	6	0
1	C	1681	0	1622	10	0
1	E	1681	0	1622	13	0
1	G	1681	0	1622	14	0
2	B	1659	0	1578	5	0
2	D	1659	0	1578	5	0
2	F	1659	0	1578	7	0
2	H	1659	0	1578	7	0
3	A	37	0	0	1	1
3	B	80	0	0	0	1
3	C	40	0	0	2	0
3	D	70	0	0	1	0
3	E	49	0	0	2	0
3	F	35	0	0	2	0
3	G	53	0	0	1	0
3	H	27	0	0	2	0
All	All	13751	0	12800	64	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (64) 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:G:130:ASP:OD2	1:G:132:THR:OG1	1.67	1.12
1:A:64:LYS:O	3:A:301:HOH:O	2.00	0.79
1:A:3:GLN:N	1:A:25:THR:O	2.17	0.77
1:C:3:GLN:N	1:C:25:THR:O	2.19	0.76
1:C:64:LYS:O	3:C:301:HOH:O	2.03	0.76
1:A:66:LYS:NZ	1:A:81:SER:O	2.21	0.73
1:G:130:ASP:OD1	1:G:132:THR:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ARG:NE	2:B:157:ASN:OD1	2.27	0.67
1:G:66:LYS:NZ	1:G:80:SER:O	2.27	0.67
1:E:130:ASP:HB3	1:E:131:THR:HA	1.75	0.67
1:C:44:GLY:O	3:C:302:HOH:O	2.14	0.65
2:F:155:ARG:O	3:F:301:HOH:O	2.14	0.65
1:E:27:TYR:O	3:E:301:HOH:O	2.15	0.64
2:H:155:ARG:NH1	3:H:302:HOH:O	2.28	0.64
1:E:66:LYS:NZ	1:E:80:SER:O	2.29	0.64
1:E:130:ASP:CB	1:E:131:THR:HA	2.31	0.61
1:C:66:LYS:NZ	1:C:80:SER:O	2.30	0.61
2:D:39:LYS:NZ	3:D:301:HOH:O	2.27	0.61
2:H:203:SER:O	3:H:301:HOH:O	2.16	0.61
1:G:130:ASP:OD2	1:G:132:THR:CB	2.56	0.54
1:C:131:THR:O	1:C:133:GLY:N	2.34	0.53
1:G:131:THR:HG22	1:G:131:THR:O	2.11	0.51
1:E:130:ASP:HB3	1:E:132:THR:H	1.75	0.51
1:E:103:TRP:CD2	2:F:44:PRO:HG2	2.46	0.51
1:E:3:GLN:N	1:E:25:THR:O	2.36	0.51
1:G:184:THR:O	1:G:187:THR:HG22	2.12	0.50
2:F:108:ARG:HD3	2:F:109:ALA:O	2.10	0.50
1:G:143:LYS:NZ	3:G:304:HOH:O	2.44	0.50
2:H:108:ARG:HD3	2:H:109:ALA:O	2.11	0.50
1:G:103:TRP:CD2	2:H:44:PRO:HG2	2.47	0.49
2:F:29:VAL:HG11	2:F:90:GLN:HG3	1.95	0.49
1:E:19:LYS:HE3	1:E:78:GLN:HE21	1.76	0.49
1:C:132:THR:HG22	1:C:132:THR:O	2.13	0.48
1:E:143:LYS:NZ	3:E:303:HOH:O	2.47	0.48
2:B:108:ARG:HD3	2:B:109:ALA:O	2.14	0.48
2:H:29:VAL:HG11	2:H:90:GLN:HG3	1.95	0.48
2:D:108:ARG:HD3	2:D:109:ALA:O	2.14	0.47
2:B:29:VAL:HG11	2:B:90:GLN:HG3	1.96	0.47
2:B:92:ASN:ND2	2:B:93:ASN:OD1	2.46	0.47
2:F:213:GLU:O	2:F:214:CYS:CB	2.63	0.47
1:E:184:THR:O	1:E:187:THR:HG22	2.16	0.46
1:E:116:PRO:HA	1:E:146:PHE:O	2.16	0.45
1:E:130:ASP:HB3	1:E:131:THR:CA	2.44	0.45
1:G:116:PRO:HA	1:G:146:PHE:O	2.16	0.45
2:D:92:ASN:ND2	2:D:93:ASN:OD1	2.49	0.44
1:C:203:SER:HB3	1:G:209:LYS:HB3	2.00	0.44
1:G:3:GLN:N	1:G:25:THR:O	2.36	0.43
2:D:29:VAL:HG11	2:D:90:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:HA	1:A:146:PHE:O	2.20	0.42
1:C:116:PRO:HA	1:C:146:PHE:O	2.20	0.42
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.02	0.42
1:A:39:GLN:HB2	1:A:45:LEU:HD23	2.03	0.41
2:D:11:MET:CE	2:D:21:VAL:HG22	2.50	0.41
2:F:70:ASP:OD2	3:F:302:HOH:O	2.22	0.41
1:E:177:LEU:HD13	1:E:178:SER:N	2.36	0.41
1:A:14:PRO:CG	1:A:113:LEU:HG	2.50	0.41
1:G:177:LEU:HD13	1:G:178:SER:N	2.36	0.41
2:H:37:GLN:HB2	2:H:47:LEU:HD11	2.03	0.40
2:H:150:ILE:HD12	2:H:155:ARG:HG3	2.02	0.40
1:C:14:PRO:CG	1:C:113:LEU:HG	2.51	0.40
1:C:39:GLN:HB2	1:C:45:LEU:HD23	2.03	0.40
1:G:125:ALA:O	1:G:213:ARG:NH1	2.50	0.40
1:G:166:PHE:O	1:G:177:LEU:HD22	2.22	0.40
2:B:11:MET:CE	2:B:21:VAL:HG22	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:301:HOH:O	3:B:337:HOH:O[2_449]	2.16	0.04

## 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	222/224 (99%)	213 (96%)	8 (4%)	1 (0%)	29 35
1	C	222/224 (99%)	214 (96%)	6 (3%)	2 (1%)	17 20
1	E	222/224 (99%)	213 (96%)	7 (3%)	2 (1%)	17 20
1	G	222/224 (99%)	215 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	212/214 (99%)	204 (96%)	8 (4%)	0	100 100
2	D	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	29 35
2	F	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
2	H	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
All	All	1736/1752 (99%)	1671 (96%)	59 (3%)	6 (0%)	41 50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	132	THR
1	C	132	THR
2	D	213	GLU
1	A	129	GLY
1	C	134	SER
1	E	129	GLY

### 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	186/186 (100%)	181 (97%)	5 (3%)	44 61
1	C	186/186 (100%)	184 (99%)	2 (1%)	73 86
1	E	186/186 (100%)	181 (97%)	5 (3%)	44 61
1	G	186/186 (100%)	182 (98%)	4 (2%)	52 69
2	B	188/188 (100%)	185 (98%)	3 (2%)	62 78
2	D	188/188 (100%)	183 (97%)	5 (3%)	44 61
2	F	188/188 (100%)	185 (98%)	3 (2%)	62 78
2	H	188/188 (100%)	185 (98%)	3 (2%)	62 78
All	All	1496/1496 (100%)	1466 (98%)	30 (2%)	55 72

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	128	CYS
1	A	132	THR
1	A	177	LEU
1	A	196	ASN
2	B	90	GLN
2	B	108	ARG
2	B	214	CYS
1	C	81	SER
1	C	177	LEU
2	D	33	LEU
2	D	90	GLN
2	D	108	ARG
2	D	212	ASN
2	D	214	CYS
1	E	132	THR
1	E	159	LEU
1	E	161	SER
1	E	177	LEU
1	E	187	THR
2	F	33	LEU
2	F	90	GLN
2	F	108	ARG
1	G	132	THR
1	G	159	LEU
1	G	177	LEU
1	G	187	THR
2	H	33	LEU
2	H	90	GLN
2	H	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	190	ASN
1	E	78	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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$
1	PCA	C	1	1	7,8,9	2.23	2 (28%)	9,10,12	2.15	5 (55%)
1	PCA	E	1	1	7,8,9	2.21	2 (28%)	9,10,12	2.08	4 (44%)
1	PCA	A	1	1	7,8,9	2.23	2 (28%)	9,10,12	2.14	5 (55%)
1	PCA	G	1	1	7,8,9	2.20	2 (28%)	9,10,12	2.07	4 (44%)

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
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	4.69	1.46	1.34
1	C	1	PCA	CD-N	4.68	1.46	1.34
1	E	1	PCA	CD-N	4.67	1.46	1.34
1	G	1	PCA	CD-N	4.64	1.46	1.34
1	A	1	PCA	CA-N	3.45	1.50	1.46
1	C	1	PCA	CA-N	3.42	1.50	1.46
1	G	1	PCA	CA-N	3.36	1.50	1.46
1	E	1	PCA	CA-N	3.35	1.50	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	PCA	CA-N-CD	-3.17	102.71	113.58
1	G	1	PCA	CA-N-CD	-3.13	102.86	113.58
1	G	1	PCA	OE-CD-CG	-3.12	121.31	126.76
1	E	1	PCA	OE-CD-CG	-3.12	121.32	126.76
1	A	1	PCA	CA-N-CD	-3.10	102.97	113.58
1	C	1	PCA	CA-N-CD	-3.10	102.98	113.58
1	A	1	PCA	OE-CD-CG	-3.09	121.38	126.76
1	C	1	PCA	OE-CD-CG	-3.07	121.40	126.76
1	C	1	PCA	CB-CA-C	-2.77	108.90	112.70
1	A	1	PCA	CB-CA-C	-2.71	108.98	112.70
1	E	1	PCA	CB-CA-N	2.55	110.63	103.30
1	G	1	PCA	CB-CA-N	2.49	110.44	103.30
1	A	1	PCA	CG-CD-N	2.44	114.71	108.39
1	E	1	PCA	CG-CD-N	2.43	114.68	108.39
1	C	1	PCA	CG-CD-N	2.43	114.68	108.39
1	G	1	PCA	CG-CD-N	2.43	114.68	108.39
1	C	1	PCA	CB-CA-N	2.42	110.25	103.30
1	A	1	PCA	CB-CA-N	2.41	110.23	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides 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	223/224 (99%)	0.17	6 (2%) 54 62	31, 57, 89, 148	0
1	C	223/224 (99%)	0.19	4 (1%) 68 74	32, 57, 90, 149	0
1	E	223/224 (99%)	0.10	4 (1%) 68 74	32, 49, 78, 129	0
1	G	223/224 (99%)	0.08	3 (1%) 77 81	31, 49, 77, 141	0
2	B	214/214 (100%)	0.05	3 (1%) 75 80	33, 46, 74, 121	0
2	D	214/214 (100%)	0.09	4 (1%) 66 73	33, 46, 73, 146	0
2	F	214/214 (100%)	0.27	8 (3%) 41 48	32, 61, 89, 136	0
2	H	214/214 (100%)	0.29	11 (5%) 28 35	35, 62, 91, 134	0
All	All	1748/1752 (99%)	0.16	43 (2%) 57 64	31, 53, 87, 149	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	THR	5.9
2	D	40	PRO	3.8
2	D	11	MET	3.8
2	F	40	PRO	3.6
1	A	130	ASP	3.3
1	E	214	GLY	3.2
2	F	62	PHE	3.1
2	F	106	ILE	3.1
2	H	106	ILE	3.1
2	B	214	CYS	3.0
2	H	40	PRO	2.8
2	F	53	TYR	2.8
2	D	214	CYS	2.7
1	G	113	LEU	2.6
2	D	41	GLY	2.6
1	A	132	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	62	PHE	2.6
1	A	2	VAL	2.5
1	E	64	LYS	2.5
1	G	132	THR	2.5
2	B	11	MET	2.5
2	H	11	MET	2.5
1	C	109	VAL	2.4
2	B	40	PRO	2.4
1	G	59	TYR	2.4
1	C	2	VAL	2.4
1	A	5	GLN	2.4
1	C	59	TYR	2.3
2	H	205	ILE	2.3
1	A	129	GLY	2.3
2	F	10	PHE	2.3
1	E	113	LEU	2.2
2	H	83	LEU	2.2
2	H	169	LYS	2.2
2	H	55	TYR	2.2
2	H	58	VAL	2.1
2	F	104	LEU	2.1
1	E	132	THR	2.1
1	A	172	SER	2.1
2	H	214	CYS	2.1
2	F	83	LEU	2.0
2	F	47	LEU	2.0
2	H	160	LEU	2.0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	A	1	8/9	0.51	0.44	67,68,69,70	0
1	PCA	G	1	8/9	0.60	0.38	45,52,55,56	0
1	PCA	E	1	8/9	0.67	0.28	50,55,57,58	0
1	PCA	C	1	8/9	0.70	0.33	60,67,69,71	0

### 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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.