



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1T4K  
Title : Crystal Structure of Unliganded Aldolase Antibody 93F3 Fab  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2004-04-29  
Resolution : 2.50 Å(reported)

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

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

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

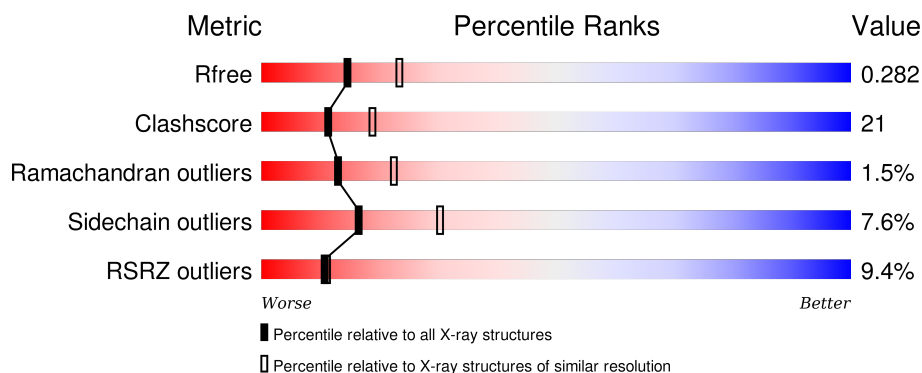
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	217	<div> <div>10%</div> <div>58%</div> <div>40%</div> <div>.</div> </div>
1	C	217	<div> <div>14%</div> <div>56%</div> <div>41%</div> <div>.</div> </div>
2	B	217	<div> <div>7%</div> <div>67%</div> <div>26%</div> <div>7%</div> </div>
2	D	217	<div> <div>6%</div> <div>64%</div> <div>30%</div> <div>6%</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
3	ZN	C	306	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6882 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 IMMUNOGLOBULIN IGG1, KAPPA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1693	1052	287	347	7			
1	C	217	Total	C	N	O	S	0	0	0
			1693	1052	287	347	7			

- Molecule 2 is a protein called IMMUNOGLOBULIN IGG1, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1605	1015	262	320	8			
2	D	217	Total	C	N	O	S	0	0	0
			1605	1015	262	320	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		
3	A	2	Total	Zn	0	0
			2	2		
3	D	1	Total	Zn	0	0
			1	1		
3	C	3	Total	Zn	0	0
			3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	74	Total	O	0	0
			74	74		

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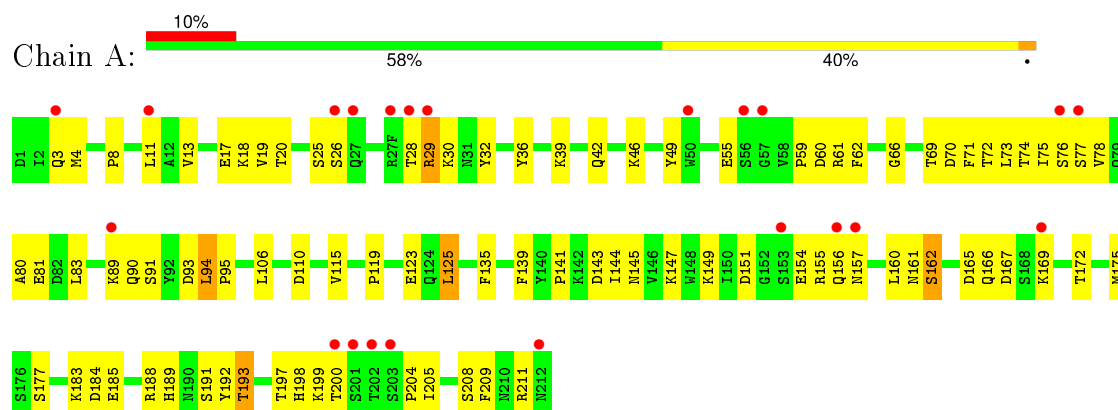
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	57	Total	O	0	0
			57	57		
4	D	83	Total	O	0	0
			83	83		

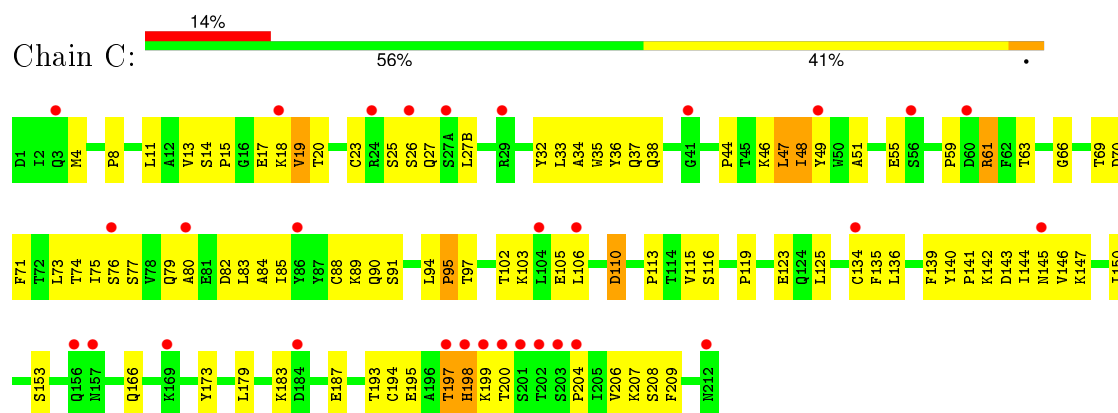
### 3 Residue-property plots

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

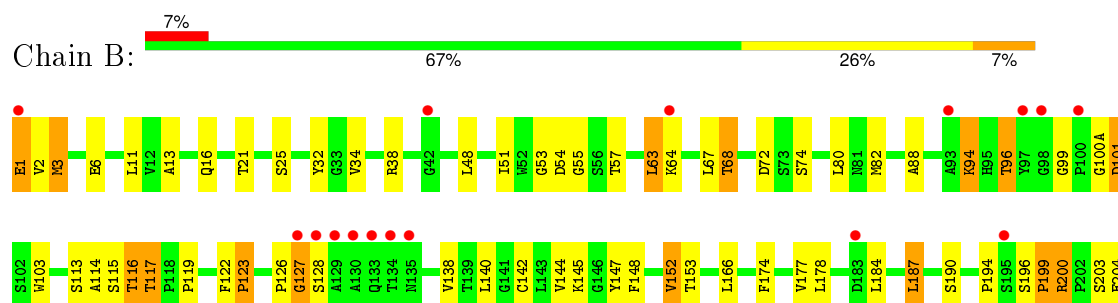
#### • Molecule 1: IMMUNOGLOBULIN IGG1, KAPPA LIGHT CHAIN



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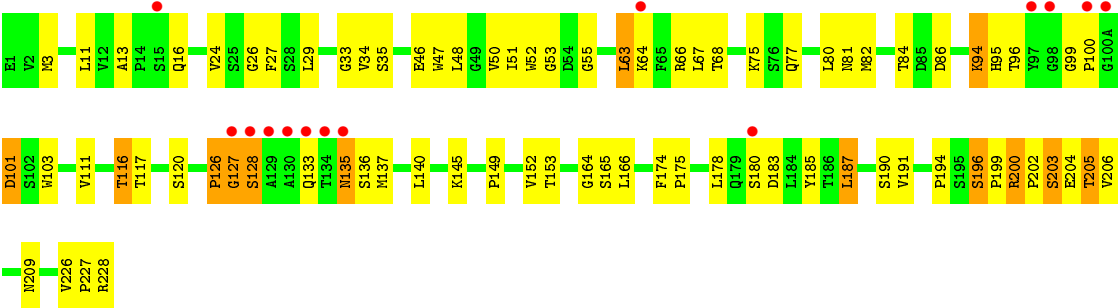


#### • Molecule 2: IMMUNOGLOBULIN IGG1, HEAVY CHAIN





● Molecule 2: IMMUNOGLOBULIN IGG1, HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.70 Å 81.23 Å 149.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.50) 89.0 (19.99-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 2.50 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.281 0.233 , 0.282	Depositor DCC
$R_{free}$ test set	1370 reflections (4.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.2	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 30651 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.4850e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: ZN

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	0.44	0/1731	0.68	0/2347
1	C	0.44	0/1731	0.66	0/2347
2	B	0.54	1/1649 (0.1%)	0.73	2/2256 (0.1%)
2	D	0.62	1/1649 (0.1%)	0.77	0/2256
All	All	0.51	2/6760 (0.0%)	0.71	2/9206 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	127	GLY	N-CA	7.61	1.57	1.46
2	B	1	GLU	CD-OE2	7.17	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	CYS	CA-CB-SG	5.28	123.51	114.00
2	B	54	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1693	0	1629	69	0
1	C	1693	0	1628	91	0
2	B	1605	0	1570	55	0
2	D	1605	0	1570	65	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	63	0	0	2	0
4	B	74	0	0	3	0
4	C	57	0	0	3	0
4	D	83	0	0	7	0
All	All	6882	0	6397	268	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 21.

All (268) 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:144:ILE:HG13	1:C:198:HIS:HB3	1.34	1.02
1:A:3:GLN:HG2	1:A:26:SER:HB3	1.43	0.99
2:D:126:PRO:O	2:D:228:ARG:HD2	1.70	0.92
2:B:194:PRO:O	2:B:199:PRO:HD2	1.72	0.88
1:A:145:ASN:HD21	1:A:197:THR:HB	1.35	0.88
1:A:80:ALA:HA	1:A:106:LEU:HD21	1.53	0.88
1:A:110:ASP:HB3	1:A:200:THR:HG22	1.58	0.84
1:C:195:GLU:HG2	1:C:206:VAL:HG22	1.59	0.84
2:D:133:GLN:HG2	2:D:135:ASN:ND2	1.96	0.80
2:B:2:VAL:O	2:B:3:MET:HG2	1.83	0.79
1:A:4:MET:HE1	1:A:90:GLN:HB3	1.65	0.78
1:C:198:HIS:CE1	1:C:200:THR:HB	2.20	0.76
1:C:183:LYS:O	1:C:187:GLU:HG3	1.85	0.76
4:C:351:HOH:O	2:D:100:PRO:HB3	1.86	0.74
2:D:95:HIS:CE1	4:D:333:HOH:O	2.41	0.74
1:C:83:LEU:HD11	1:C:166:GLN:HB3	1.70	0.73
2:B:113:SER:OG	2:D:26:GLY:HA2	1.89	0.73
2:B:51:ILE:HD12	2:B:57:THR:HG22	1.71	0.73
1:C:206:VAL:O	1:C:207:LYS:HD2	1.88	0.72
1:A:193:THR:HB	1:A:208:SER:HB3	1.72	0.71
2:D:194:PRO:HB2	2:D:199:PRO:HD2	1.73	0.71
2:D:47:TRP:CZ2	2:D:50:VAL:HG23	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:O	1:C:106:LEU:HD12	1.93	0.68
2:B:3:MET:HB2	2:B:25:SER:HB2	1.75	0.68
1:C:197:THR:OG1	1:C:204:PRO:HB3	1.94	0.68
2:D:200:ARG:HD2	2:D:202:PRO:HA	1.75	0.68
1:C:20:THR:HG22	1:C:74:THR:OG1	1.94	0.67
2:D:35:SER:CB	2:D:50:VAL:HG22	2.24	0.67
2:D:133:GLN:HG2	2:D:135:ASN:HD22	1.58	0.66
2:B:127:GLY:O	2:B:128:SER:HB3	1.94	0.66
1:C:193:THR:HG23	1:C:208:SER:HB2	1.75	0.66
2:B:48:LEU:HD22	2:B:63:LEU:HD21	1.75	0.66
2:D:47:TRP:HZ2	2:D:50:VAL:HG23	1.60	0.66
2:D:153:THR:HG22	4:D:339:HOH:O	1.96	0.65
1:A:192:TYR:O	1:A:208:SER:HB2	1.97	0.65
1:A:151:ASP:HA	1:A:191:SER:HB3	1.78	0.65
1:C:144:ILE:HG13	1:C:198:HIS:CB	2.20	0.64
2:B:205:THR:HG22	4:B:323:HOH:O	1.97	0.64
1:A:39:LYS:HB2	1:A:42:GLN:HE21	1.62	0.64
1:A:145:ASN:ND2	1:A:197:THR:HB	2.10	0.64
2:B:196:SER:HB2	2:B:199:PRO:HD3	1.79	0.63
1:A:188:ARG:O	2:D:199:PRO:HG2	1.98	0.62
2:B:178:LEU:HD12	2:B:184:LEU:O	1.99	0.62
2:D:33:GLY:HA3	2:D:52:TRP:CE3	2.33	0.62
1:A:160:LEU:HB3	2:B:177:VAL:HG21	1.81	0.62
2:D:67:LEU:HD11	2:D:80:LEU:HD11	1.83	0.61
1:C:63:THR:CG2	1:C:74:THR:HB	2.30	0.61
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.36	0.61
2:B:199:PRO:O	2:B:204:GLU:N	2.33	0.60
1:C:119:PRO:HB3	1:C:209:PHE:CE1	2.36	0.60
1:A:110:ASP:OD2	1:A:199:LYS:HE3	2.02	0.60
1:C:103:LYS:HD2	1:C:105:GLU:HG3	1.84	0.59
1:C:119:PRO:HB3	1:C:209:PHE:CZ	2.37	0.59
2:D:68:THR:HG23	2:D:81:ASN:HB2	1.82	0.59
1:A:167:ASP:OD1	1:A:169:LYS:HB2	2.02	0.59
2:D:187:LEU:HD12	2:D:187:LEU:C	2.23	0.59
1:C:48:ILE:HD11	1:C:51:ALA:O	2.03	0.58
1:C:33:LEU:C	1:C:33:LEU:HD23	2.22	0.58
2:B:13:ALA:O	2:B:16:GLN:HB2	2.03	0.58
1:C:115:VAL:HB	1:C:207:LYS:HG3	1.85	0.58
1:A:18:LYS:HB2	1:A:76:SER:O	2.04	0.58
1:C:17:GLU:O	1:C:77:SER:HA	2.04	0.58
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.85	0.57
1:C:85:ILE:HD12	1:C:102:THR:C	2.25	0.57
1:C:15:PRO:HD3	1:C:106:LEU:HD11	1.87	0.57
2:B:94:LYS:O	2:B:101:ASP:HA	2.05	0.57
1:A:13:VAL:CG1	1:A:78:VAL:HG21	2.34	0.57
1:A:13:VAL:HG11	1:A:78:VAL:HG21	1.86	0.56
2:D:196:SER:CB	2:D:199:PRO:HD3	2.36	0.56
1:C:8:PRO:CG	1:C:11:LEU:HG	2.35	0.56
1:C:80:ALA:HA	1:C:106:LEU:HD22	1.88	0.56
1:C:25:SER:O	1:C:69:THR:HG23	2.06	0.55
1:C:135:PHE:CE2	2:D:190:SER:HB3	2.40	0.55
2:B:80:LEU:HD21	2:B:82:MET:HG3	1.86	0.55
1:A:185:GLU:OE2	1:A:189:HIS:NE2	2.40	0.55
1:C:197:THR:HG23	1:C:204:PRO:HB3	1.88	0.55
2:D:11:LEU:HD23	2:D:116:THR:HG22	1.88	0.55
1:A:13:VAL:HG22	1:A:17:GLU:HB2	1.88	0.55
2:D:94:LYS:O	2:D:101:ASP:HA	2.07	0.55
2:B:144:VAL:HB	2:B:187:LEU:HD22	1.89	0.55
1:A:169:LYS:HD3	4:A:334:HOH:O	2.06	0.55
2:B:194:PRO:C	2:B:199:PRO:HD2	2.28	0.54
1:C:35:TRP:HB2	1:C:48:ILE:HG23	1.88	0.54
1:C:4:MET:HE3	1:C:23:CYS:SG	2.47	0.54
1:A:139:PHE:O	1:A:172:THR:HB	2.08	0.54
1:A:125:LEU:HD12	1:A:183:LYS:HG3	1.89	0.54
2:D:194:PRO:HB2	2:D:199:PRO:CD	2.36	0.54
2:D:13:ALA:O	2:D:16:GLN:HB2	2.08	0.54
1:A:61:ARG:O	1:A:75:ILE:HA	2.08	0.54
2:D:84:THR:HA	2:D:111:VAL:HB	1.89	0.54
1:C:75:ILE:HD12	1:C:75:ILE:N	2.23	0.54
1:C:125:LEU:O	1:C:183:LYS:HD2	2.06	0.54
1:C:79:GLN:NE2	4:C:321:HOH:O	2.40	0.54
1:C:13:VAL:HG11	1:C:19:VAL:HG11	1.89	0.53
1:A:184:ASP:O	1:A:188:ARG:HG3	2.09	0.53
1:A:193:THR:HB	1:A:208:SER:CB	2.38	0.53
2:D:178:LEU:HB2	2:D:185:TYR:CE1	2.43	0.53
2:D:226:VAL:HG22	4:D:310:HOH:O	2.07	0.53
2:D:95:HIS:CD2	2:D:96:THR:H	2.27	0.53
2:D:35:SER:OG	2:D:50:VAL:HG22	2.09	0.53
1:C:150:ILE:HD11	1:C:179:LEU:HD21	1.91	0.53
2:D:66:ARG:NH2	2:D:86:ASP:OD2	2.42	0.52
2:B:115:SER:O	2:B:117:THR:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:HD3	1:A:154:GLU:OE1	2.10	0.52
2:D:180:SER:O	2:D:183:ASP:HB2	2.10	0.52
1:C:8:PRO:HG2	1:C:11:LEU:HG	1.92	0.52
1:A:17:GLU:O	1:A:77:SER:HA	2.11	0.51
1:A:83:LEU:HD11	1:A:166:GLN:HB3	1.90	0.51
1:A:141:PRO:HD2	1:A:198:HIS:CE1	2.45	0.51
2:B:80:LEU:C	2:B:80:LEU:HD23	2.30	0.51
1:C:38:GLN:HB3	1:C:85:ILE:HG23	1.91	0.51
2:D:194:PRO:O	2:D:199:PRO:HD2	2.10	0.51
1:A:25:SER:O	1:A:69:THR:HG23	2.10	0.51
2:B:11:LEU:HD23	2:B:116:THR:HG22	1.92	0.51
1:A:32:TYR:HB3	1:A:91:SER:HB2	1.93	0.51
2:B:103:TRP:N	2:B:103:TRP:CD1	2.79	0.51
1:A:59:PRO:HG2	1:A:62:PHE:CD2	2.47	0.50
1:C:142:LYS:HB2	1:C:173:TYR:CE1	2.46	0.50
1:A:184:ASP:HB2	2:D:165:SER:OG	2.12	0.50
1:C:103:LYS:HD2	1:C:105:GLU:CG	2.41	0.50
1:C:48:ILE:HD11	1:C:51:ALA:C	2.32	0.50
1:C:90:GLN:HE21	1:C:97:THR:HB	1.77	0.50
2:D:51:ILE:HG23	2:D:51:ILE:O	2.12	0.50
1:C:20:THR:HA	1:C:73:LEU:O	2.12	0.50
1:C:27(B):LEU:HD12	1:C:71:PHE:CE1	2.46	0.50
1:C:139:PHE:CE2	1:C:144:ILE:HB	2.47	0.50
1:A:8:PRO:HG2	1:A:11:LEU:HG	1.93	0.50
2:D:35:SER:HB3	2:D:50:VAL:HG22	1.94	0.49
1:C:18:LYS:HB2	1:C:76:SER:O	2.12	0.49
1:C:83:LEU:C	1:C:83:LEU:HD23	2.33	0.49
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.94	0.49
1:C:197:THR:CG2	1:C:204:PRO:HB3	2.43	0.49
1:C:36:TYR:HE2	1:C:89:LYS:HD3	1.78	0.49
2:B:119:PRO:HB2	2:B:144:VAL:HG13	1.95	0.49
2:D:33:GLY:HA3	2:D:52:TRP:CZ3	2.48	0.48
2:D:48:LEU:HD22	2:D:63:LEU:HD21	1.95	0.48
2:B:126:PRO:HD3	2:B:140:LEU:CD1	2.44	0.48
1:C:115:VAL:HB	1:C:207:LYS:CG	2.43	0.48
1:C:13:VAL:HG11	1:C:19:VAL:CG1	2.43	0.48
2:D:11:LEU:HB2	2:D:149:PRO:HG3	1.96	0.48
2:B:144:VAL:HB	2:B:187:LEU:CD2	2.43	0.48
1:A:162:SER:O	1:A:175:MET:HA	2.13	0.48
2:D:135:ASN:OD1	2:D:137:MET:O	2.32	0.47
1:A:149:LYS:NZ	4:A:348:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TYR:CD1	2:B:96:THR:HG23	2.49	0.47
1:C:8:PRO:HG3	1:C:11:LEU:HG	1.97	0.47
2:D:68:THR:CG2	2:D:81:ASN:HB2	2.43	0.47
1:C:4:MET:CE	1:C:90:GLN:HB3	2.44	0.47
1:A:78:VAL:O	1:A:78:VAL:HG23	2.15	0.47
2:D:46:GLU:HA	4:D:343:HOH:O	2.15	0.47
1:A:66:GLY:HA3	1:A:71:PHE:HA	1.97	0.47
2:B:187:LEU:HA	4:B:339:HOH:O	2.14	0.47
1:C:61:ARG:NH2	1:C:82:ASP:OD1	2.47	0.47
2:B:178:LEU:HD21	4:B:378:HOH:O	2.15	0.47
2:D:127:GLY:O	2:D:128:SER:HB2	2.15	0.47
1:A:20:THR:HA	1:A:73:LEU:O	2.14	0.46
1:C:110:ASP:OD2	1:C:199:LYS:HG2	2.15	0.46
1:C:26:SER:C	1:C:27:GLN:HG3	2.35	0.46
1:C:135:PHE:CZ	2:D:190:SER:HB3	2.50	0.46
1:C:66:GLY:HA3	1:C:71:PHE:HA	1.97	0.46
2:D:95:HIS:ND1	4:D:370:HOH:O	2.35	0.46
1:C:46:LYS:HD3	1:C:49:TYR:HB3	1.97	0.46
1:A:149:LYS:O	1:A:193:THR:HG23	2.16	0.46
1:C:33:LEU:HD23	1:C:34:ALA:N	2.30	0.46
1:C:34:ALA:O	1:C:88:CYS:HA	2.16	0.46
1:C:141:PRO:HB2	1:C:143:ASP:OD1	2.15	0.46
1:A:28:THR:O	1:A:30:LYS:HG2	2.15	0.46
2:D:199:PRO:O	2:D:204:GLU:N	2.40	0.46
2:B:114:ALA:HB3	2:B:148:PHE:CE2	2.51	0.45
1:C:20:THR:HG22	1:C:74:THR:HG23	1.97	0.45
1:C:61:ARG:O	1:C:75:ILE:HA	2.16	0.45
2:B:152:VAL:HG12	2:B:187:LEU:HD13	1.98	0.45
1:C:37:GLN:HB2	1:C:47:LEU:HD22	1.97	0.45
1:C:49:TYR:CE2	2:D:99:GLY:HA2	2.51	0.45
2:D:202:PRO:HG3	2:D:227:PRO:HG3	1.98	0.45
2:D:145:LYS:HB2	2:D:145:LYS:HE3	1.75	0.45
1:C:195:GLU:CG	1:C:206:VAL:HG22	2.40	0.45
1:C:83:LEU:O	1:C:84:ALA:HB2	2.17	0.45
1:A:144:ILE:HB	1:A:198:HIS:HD2	1.81	0.45
2:B:53:GLY:C	2:B:55:GLY:H	2.20	0.45
2:B:122:PHE:HA	2:B:123:PRO:HD3	1.76	0.45
1:A:8:PRO:CG	1:A:11:LEU:HG	2.47	0.45
2:D:86:ASP:HB2	2:D:111:VAL:HG21	1.99	0.45
1:C:59:PRO:HB2	1:C:61:ARG:HD3	1.99	0.45
1:C:32:TYR:HB3	1:C:91:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:THR:OG1	1:A:204:PRO:HB3	2.17	0.44
1:A:20:THR:HG22	1:A:74:THR:OG1	2.17	0.44
2:D:34:VAL:O	2:D:51:ILE:HG22	2.17	0.44
2:B:67:LEU:HD12	2:B:68:THR:N	2.32	0.44
1:C:46:LYS:HE2	4:D:330:HOH:O	2.17	0.44
1:A:49:TYR:CE2	2:B:99:GLY:HA2	2.53	0.44
2:B:72:ASP:OD1	2:B:74:SER:HB2	2.17	0.44
2:B:38:ARG:HG3	2:B:88:ALA:HB3	2.00	0.44
1:C:63:THR:HG23	1:C:74:THR:HB	1.99	0.44
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.52	0.44
1:A:89:LYS:HE3	1:A:95:PRO:HB3	2.00	0.44
2:D:67:LEU:HD12	2:D:82:MET:HG2	1.99	0.44
1:A:157:ASN:HD22	1:A:157:ASN:N	2.14	0.44
1:A:157:ASN:ND2	1:A:157:ASN:N	2.66	0.44
1:A:36:TYR:CE1	1:A:46:LYS:HB2	2.53	0.44
1:A:141:PRO:HD2	1:A:198:HIS:HE1	1.83	0.43
1:C:95:PRO:HB2	2:D:47:TRP:CG	2.53	0.43
1:C:197:THR:CB	1:C:204:PRO:HB3	2.48	0.43
1:C:63:THR:HG22	1:C:74:THR:HB	1.99	0.43
2:B:194:PRO:HB2	2:B:199:PRO:CD	2.48	0.43
2:B:196:SER:CB	2:B:199:PRO:HD3	2.47	0.43
1:A:135:PHE:CE2	2:B:190:SER:HB3	2.54	0.43
2:B:200:ARG:HB3	2:B:200:ARG:HE	1.34	0.43
2:B:138:VAL:HG13	2:B:138:VAL:O	2.17	0.43
2:B:174:PHE:CD1	2:B:174:PHE:N	2.86	0.43
1:C:193:THR:HG22	1:C:194:CYS:N	2.33	0.43
2:B:187:LEU:C	2:B:187:LEU:HD23	2.39	0.43
2:D:24:VAL:HB	2:D:27:PHE:CZ	2.54	0.43
1:C:115:VAL:HA	1:C:135:PHE:O	2.19	0.43
1:C:47:LEU:HB3	1:C:48:ILE:HG22	1.99	0.43
2:B:2:VAL:C	2:B:3:MET:HG2	2.39	0.43
1:A:205:ILE:N	1:A:205:ILE:HD12	2.34	0.43
1:C:146:VAL:O	1:C:147:LYS:HD2	2.18	0.43
2:B:51:ILE:HD12	2:B:57:THR:CG2	2.44	0.43
1:C:63:THR:O	1:C:63:THR:HG23	2.19	0.43
2:D:187:LEU:CD1	2:D:187:LEU:C	2.87	0.43
2:B:6:GLU:HA	2:B:21:THR:O	2.19	0.43
2:B:34:VAL:O	2:B:51:ILE:HG22	2.19	0.43
1:C:38:GLN:HB2	1:C:44:PRO:HG3	2.00	0.43
1:C:18:LYS:HG3	1:C:75:ILE:O	2.19	0.43
2:D:166:LEU:HD22	2:D:191:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:HD22	1:A:177:SER:HA	1.84	0.43
1:A:29:ARG:HH11	1:A:29:ARG:CG	2.32	0.42
1:C:15:PRO:CD	1:C:106:LEU:HD11	2.49	0.42
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.84	0.42
1:C:193:THR:CG2	1:C:208:SER:HB2	2.47	0.42
1:A:8:PRO:HG3	1:A:11:LEU:HD21	2.00	0.42
2:D:164:GLY:HA2	4:D:317:HOH:O	2.18	0.42
2:D:24:VAL:HG21	2:D:29:LEU:HD21	2.01	0.42
1:C:116:SER:O	1:C:134:CYS:HA	2.19	0.42
2:D:196:SER:HB2	2:D:199:PRO:HD3	2.01	0.42
2:D:75:LYS:O	2:D:77:GLN:HG3	2.19	0.42
1:A:119:PRO:HG2	2:B:228:ARG:NH2	2.34	0.42
1:A:69:THR:CG2	1:A:69:THR:O	2.67	0.42
1:C:136:LEU:HD21	1:C:146:VAL:HG22	2.01	0.42
1:C:46:LYS:HE3	2:D:101:ASP:CB	2.49	0.42
1:C:200:THR:HG23	4:C:313:HOH:O	2.18	0.41
1:C:14:SER:O	1:C:17:GLU:HG3	2.20	0.41
1:C:36:TYR:CE1	1:C:46:LYS:HB2	2.55	0.41
1:A:19:VAL:HG22	1:A:78:VAL:HG11	2.00	0.41
1:A:13:VAL:CG2	1:A:17:GLU:HB2	2.49	0.41
1:C:140:TYR:CG	1:C:141:PRO:HA	2.55	0.41
1:A:115:VAL:HA	1:A:135:PHE:O	2.19	0.41
2:D:103:TRP:CD1	2:D:103:TRP:N	2.85	0.41
2:D:53:GLY:C	2:D:55:GLY:N	2.73	0.41
2:B:94:LYS:HD3	2:B:94:LYS:C	2.41	0.41
2:D:174:PHE:HA	2:D:175:PRO:HD3	1.90	0.41
2:B:194:PRO:HD2	2:B:199:PRO:HG2	2.03	0.41
2:B:100(A):GLY:O	2:B:101:ASP:C	2.59	0.41
2:B:123:PRO:HG3	2:B:221:LYS:HD2	2.01	0.41
1:A:156:GLN:HG3	1:A:157:ASN:ND2	2.35	0.41
1:C:139:PHE:HE2	1:C:144:ILE:HB	1.86	0.41
1:A:197:THR:HA	1:A:204:PRO:HB3	2.02	0.41
2:D:67:LEU:CD1	2:D:80:LEU:HD11	2.49	0.41
1:A:211:ARG:HB3	1:A:211:ARG:NH1	2.36	0.41
2:B:127:GLY:O	2:B:128:SER:CB	2.68	0.41
2:B:67:LEU:HD12	2:B:68:THR:H	1.85	0.41
1:A:93:ASP:O	1:A:94:LEU:O	2.39	0.40
2:D:200:ARG:HB3	2:D:200:ARG:HE	1.45	0.40
1:A:197:THR:CB	1:A:204:PRO:HB3	2.52	0.40
2:B:53:GLY:C	2:B:55:GLY:N	2.74	0.40
2:D:205:THR:HG23	2:D:206:VAL:N	2.36	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	215/217 (99%)	195 (91%)	18 (8%)	2 (1%)	21	37
1	C	215/217 (99%)	198 (92%)	15 (7%)	2 (1%)	21	37
2	B	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	8	12
2	D	215/217 (99%)	198 (92%)	13 (6%)	4 (2%)	10	16
All	All	860/868 (99%)	783 (91%)	64 (7%)	13 (2%)	13	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	ASP
2	B	101	ASP
2	B	127	GLY
2	B	203	SER
2	D	101	ASP
2	D	203	SER
2	D	64	LYS
2	D	128	SER
1	A	94	LEU
2	B	64	LYS
1	C	94	LEU
1	C	95	PRO
2	B	199	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/195 (100%)	183 (94%)	12 (6%)	23	41
1	C	195/195 (100%)	183 (94%)	12 (6%)	23	41
2	B	186/186 (100%)	169 (91%)	17 (9%)	12	22
2	D	186/186 (100%)	169 (91%)	17 (9%)	12	22
All	All	762/762 (100%)	704 (92%)	58 (8%)	16	30

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	55	GLU
1	A	60	ASP
1	A	70	ASP
1	A	72	THR
1	A	81	GLU
1	A	123	GLU
1	A	125	LEU
1	A	155	ARG
1	A	162	SER
1	A	165	ASP
1	A	193	THR
2	B	1	GLU
2	B	3	MET
2	B	63	LEU
2	B	68	THR
2	B	94	LYS
2	B	96	THR
2	B	116	THR
2	B	117	THR
2	B	123	PRO
2	B	145	LYS
2	B	152	VAL
2	B	153	THR
2	B	166	LEU
2	B	187	LEU
2	B	200	ARG
2	B	209	ASN
2	B	227	PRO
1	C	19	VAL

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Mol	Chain	Res	Type
1	C	47	LEU
1	C	48	ILE
1	C	55	GLU
1	C	61	ARG
1	C	70	ASP
1	C	110	ASP
1	C	123	GLU
1	C	145	ASN
1	C	153	SER
1	C	197	THR
1	C	198	HIS
2	D	3	MET
2	D	63	LEU
2	D	94	LYS
2	D	116	THR
2	D	117	THR
2	D	120	SER
2	D	126	PRO
2	D	135	ASN
2	D	136	SER
2	D	140	LEU
2	D	152	VAL
2	D	187	LEU
2	D	196	SER
2	D	200	ARG
2	D	203	SER
2	D	205	THR
2	D	209	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	137	ASN
1	A	145	ASN
1	A	161	ASN
1	A	212	ASN
2	B	81	ASN
2	B	83(C)	GLN
2	B	95	HIS
2	B	179	GLN
1	C	27	GLN

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Mol	Chain	Res	Type
1	C	90	GLN
1	C	210	ASN
1	C	212	ASN
2	D	83	HIS
2	D	135	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	217/217 (100%)	0.47	22 (10%) 9 9	27, 54, 82, 100	0
1	C	217/217 (100%)	0.89	30 (13%) 4 4	32, 65, 88, 110	0
2	B	217/217 (100%)	0.42	16 (7%) 17 19	23, 40, 85, 108	0
2	D	217/217 (100%)	0.42	14 (6%) 22 25	23, 43, 84, 109	0
All	All	868/868 (100%)	0.55	82 (9%) 11 11	23, 50, 86, 110	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	129	ALA	14.2
2	D	130	ALA	12.0
2	B	130	ALA	11.4
2	D	129	ALA	11.3
2	B	97	TYR	10.2
2	B	128	SER	9.2
2	D	97	TYR	9.2
2	D	128	SER	9.1
2	D	134	THR	8.1
1	A	202	THR	6.7
2	B	133	GLN	6.5
1	C	200	THR	6.4
2	D	133	GLN	6.4
1	C	201	SER	6.2
2	B	135	ASN	5.4
2	B	127	GLY	5.0
2	D	98	GLY	4.9
2	B	100	PRO	4.6
2	B	64	LYS	4.6
2	D	64	LYS	4.5
2	D	135	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	169	LYS	4.4
1	C	203	SER	4.3
1	C	56	SER	4.0
1	C	198	HIS	3.9
1	A	27(F)	ARG	3.8
1	A	56	SER	3.8
2	D	127	GLY	3.7
1	A	3	GLN	3.7
1	C	29	ARG	3.6
1	C	212	ASN	3.5
1	C	26	SER	3.5
1	A	76	SER	3.4
1	C	41	GLY	3.4
1	C	3	GLN	3.3
1	C	199	LYS	3.3
1	A	156	GLN	3.2
1	A	157	ASN	3.1
1	C	106	LEU	3.0
1	A	153	SER	3.0
1	C	145	ASN	3.0
2	B	134	THR	3.0
2	B	42	GLY	3.0
2	D	100(A)	GLY	2.9
1	C	169	LYS	2.8
1	A	26	SER	2.8
1	C	49	TYR	2.7
1	A	201	SER	2.7
2	B	98	GLY	2.7
1	C	80	ALA	2.7
1	A	77	SER	2.7
1	C	197	THR	2.7
1	A	29	ARG	2.6
1	C	184	ASP	2.6
1	C	202	THR	2.5
1	C	27(A)	SER	2.5
1	C	86	TYR	2.5
2	B	1	GLU	2.5
1	A	28	THR	2.5
1	A	203	SER	2.5
2	D	15	SER	2.5
1	A	27	GLN	2.4
2	D	180	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	24	ARG	2.4
2	B	93	ALA	2.4
2	D	100	PRO	2.4
2	B	195	SER	2.4
1	C	134	CYS	2.3
1	C	60	ASP	2.3
1	C	18	LYS	2.3
1	A	57	GLY	2.3
1	A	50	TRP	2.3
1	C	204	PRO	2.3
1	C	156	GLN	2.2
1	C	157	ASN	2.2
1	A	212	ASN	2.2
2	B	183	ASP	2.2
1	C	104	LEU	2.1
1	C	76	SER	2.1
1	A	11	LEU	2.0
1	A	200	THR	2.0
1	A	89	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
3	ZN	C	306	1/1	0.97	0.54	5.77	66,66,66,66	1
3	ZN	A	304	1/1	0.95	0.17	0.38	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	305	1/1	0.83	0.10	-1.00	64,64,64,64	1
3	ZN	B	308	1/1	0.98	0.07	-1.19	50,50,50,50	0
3	ZN	C	301	1/1	0.91	0.07	-2.03	61,61,61,61	1
3	ZN	D	307	1/1	0.92	0.14	-	65,65,65,65	1
3	ZN	C	302	1/1	0.80	0.36	-	69,69,69,69	1
3	ZN	B	309	1/1	0.88	0.08	-	54,54,54,54	1
3	ZN	B	303	1/1	0.97	0.10	-	61,61,61,61	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.