



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:43 am BST

PDB ID : 6CW3  
Title : Crystal structure of a yeast SAGA transcriptional coactivator Ada2/Gcn5 HAT subcomplex, crystal form 2  
Authors : Sun, J.; Paduch, M.; Kim, S.A.; Kramer, R.M.; Barrios, A.F.; Lu, V.; Luke, J.; Usatyuk, S.; Kossiakoff, A.A.; Tan, S.  
Deposited on : 2018-03-29  
Resolution : 1.98 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 ⓘ 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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

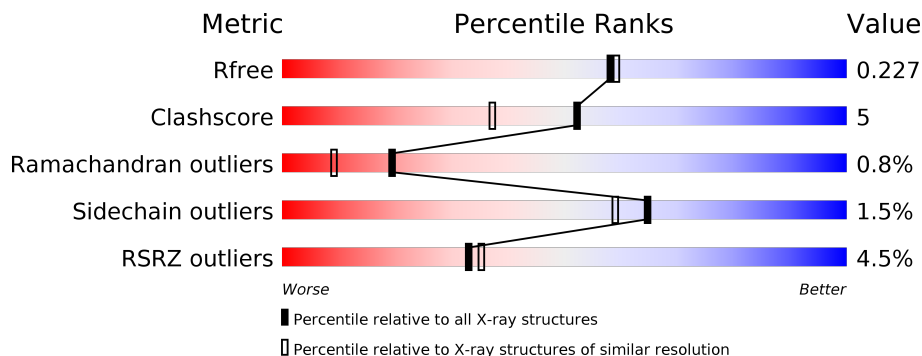
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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.



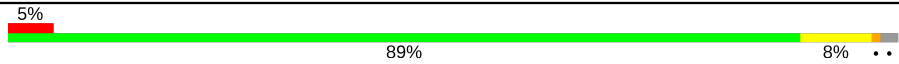

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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  $\leq 5\%$ . 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	234	88% (6% • 5%)
1	C	234	91% (• 6%)
2	B	215	91% (8% •)
2	D	215	91% (8% •)
3	F	254	7% (63% 15% • 22%)
3	H	254	9% (57% 17% • 25%)

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Mol	Chain	Length	Quality of chain
4	E	122	 <p>5% 89% 8% ..</p>
4	G	122	 <p>11% 51% 20% 5% 25%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11837 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total	C	N	O	S	0	0	0
			1663	1056	272	328	7			
1	C	220	Total	C	N	O	S	0	0	0
			1662	1057	272	324	9			

- Molecule 2 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total	C	N	O	S	0	0	0
			1613	1010	274	324	5			
2	D	213	Total	C	N	O	S	0	0	0
			1620	1013	274	328	5			

- Molecule 3 is a protein called Histone acetyltransferase GCN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	199	Total	C	N	O	S	0	0	0
			1535	990	268	267	10			
3	H	191	Total	C	N	O	S	0	0	0
			1448	933	253	256	6			

- Molecule 4 is a protein called Transcriptional adapter 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	120	Total	C	N	O	S	0	0	0
			940	595	155	182	8			
4	G	92	Total	C	N	O	S	0	0	0
			690	441	118	124	7			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	119	Total	O	0	0
			119	119		
6	B	130	Total	O	0	0
			130	130		
6	C	155	Total	O	0	0
			155	155		
6	D	147	Total	O	0	0
			147	147		
6	F	49	Total	O	0	0
			49	49		
6	E	18	Total	O	0	0
			18	18		
6	H	23	Total	O	0	0
			23	23		
6	G	21	Total	O	0	0
			21	21		

### 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: antibody heavy chain

Chain A: 

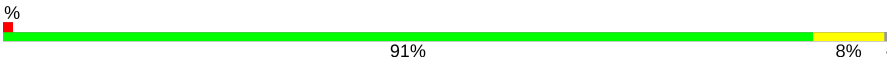


- Molecule 1: antibody heavy chain

Chain C: 



- Molecule 2: antibody light chain

Chain B: 



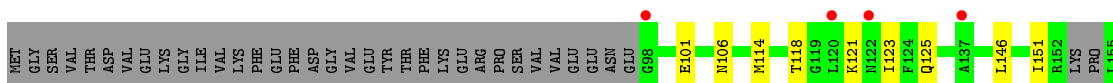
- Molecule 2: antibody light chain

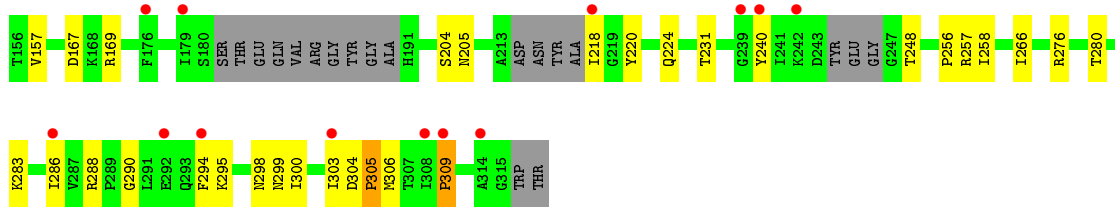
Chain D: 



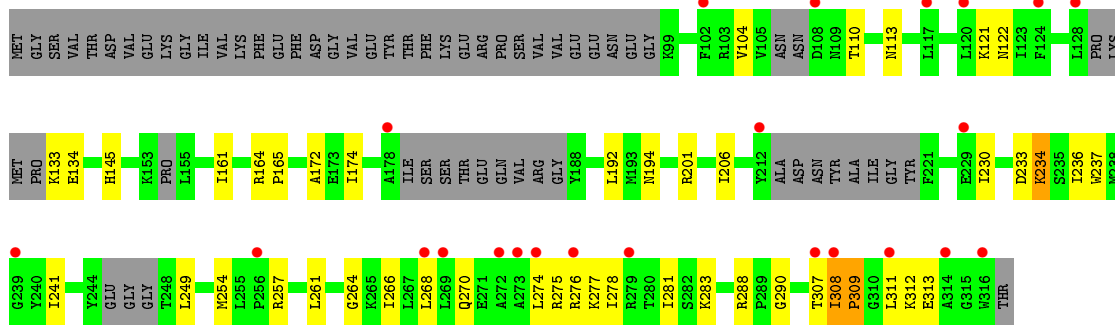
- Molecule 3: Histone acetyltransferase GCN5

Chain F: 

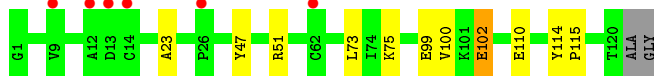
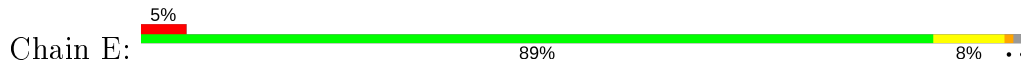




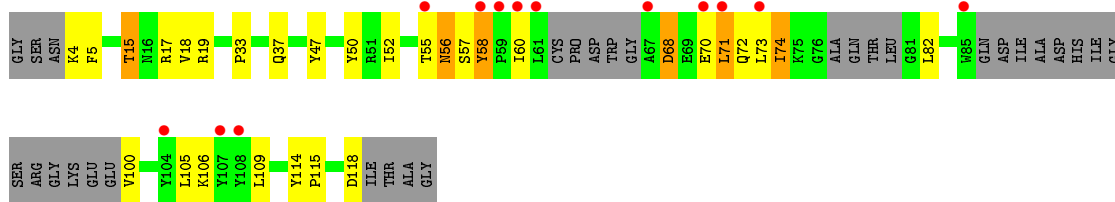
• Molecule 3: Histone acetyltransferase GCN5



• Molecule 4: Transcriptional adapter 2



• Molecule 4: Transcriptional adapter 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.66Å 104.06Å 166.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.22 – 1.98 88.22 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (88.22-1.98) 99.9 (88.22-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.203 , 0.227 0.203 , 0.227	Depositor DCC
$R_{free}$ test set	6047 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtrriage
Anisotropy	0.096	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.036 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.43	0/1708	0.55	0/2332
1	C	0.48	0/1707	0.57	0/2326
2	B	0.41	0/1647	0.57	0/2238
2	D	0.45	0/1654	0.59	0/2247
3	F	0.33	0/1561	0.53	0/2104
3	H	0.32	0/1469	0.57	0/1983
4	E	0.34	0/966	0.52	0/1315
4	G	0.40	0/708	0.61	1/965 (0.1%)
All	All	0.40	0/11420	0.56	1/15510 (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
4	G	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	71	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	70	GLU	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	1663	0	1576	7	0
1	C	1662	0	1596	3	0
2	B	1613	0	1559	12	0
2	D	1620	0	1574	13	0
3	F	1535	0	1513	29	0
3	H	1448	0	1386	34	0
4	E	940	0	868	8	0
4	G	690	0	601	25	0
5	E	2	0	0	0	0
5	G	2	0	0	0	0
6	A	119	0	0	2	0
6	B	130	0	0	2	0
6	C	155	0	0	1	0
6	D	147	0	0	1	0
6	E	18	0	0	0	0
6	F	49	0	0	5	0
6	G	21	0	0	2	0
6	H	23	0	0	1	0
All	All	11837	0	10673	120	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 5.

All (120) 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:B:25:ARG:NH2	2:B:71:ASP:OD2	1.99	0.94
3:F:304:ASP:O	3:F:306:MET:N	2.09	0.86
4:G:56:ASN:OD1	4:G:57:SER:N	2.09	0.85
4:G:19:ARG:NH2	6:G:302:HOH:O	2.18	0.75
3:H:104:VAL:O	6:H:401:HOH:O	2.06	0.73
4:G:118:ASP:OD2	6:G:301:HOH:O	2.06	0.73
3:F:256:PRO:O	6:F:401:HOH:O	2.07	0.73
2:B:3:ILE:HD13	2:D:5:MET:HA	1.74	0.69
4:G:33:PRO:O	4:G:37:GLN:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:172:ALA:HB2	3:H:206:ILE:HD13	1.75	0.67
3:F:305:PRO:O	6:F:402:HOH:O	2.12	0.67
1:A:147:GLY:N	6:A:301:HOH:O	2.28	0.66
2:B:32:SER:O	2:B:67:ARG:NH2	2.26	0.66
2:D:32:SER:O	2:D:67:ARG:NH1	2.28	0.66
4:G:71:LEU:H	4:G:74:ILE:HG12	1.63	0.63
4:G:5:PHE:H	4:G:15:THR:HG23	1.65	0.62
3:H:308:ILE:HB	3:H:309:PRO:HD3	1.81	0.62
3:F:288:ARG:HG3	3:F:309:PRO:HG3	1.80	0.61
1:A:222:LYS:NZ	6:A:302:HOH:O	2.29	0.61
2:D:30:VAL:HG13	3:F:205:ASN:HB2	1.83	0.61
3:F:257:ARG:NH1	4:E:110:GLU:OE2	2.34	0.61
2:D:106:GLU:HG3	2:D:174:TYR:OH	2.02	0.60
3:F:298:ASN:ND2	6:F:405:HOH:O	2.35	0.59
3:F:218:ILE:HD11	3:F:248:THR:HG21	1.86	0.58
4:E:73:LEU:HD13	4:E:100:VAL:HG13	1.85	0.58
3:F:294:PHE:CE1	3:F:300:ILE:HG23	2.38	0.58
2:D:2:ASP:N	2:D:2:ASP:OD2	2.36	0.57
2:D:146:LYS:HG2	2:D:198:THR:HB	1.85	0.57
3:H:281:ILE:HD13	4:G:58:TYR:HE2	1.68	0.57
4:G:50:TYR:HE2	4:G:52:ILE:HD11	1.71	0.55
3:F:231:THR:HG23	6:F:404:HOH:O	2.06	0.55
4:G:71:LEU:HG	4:G:72:GLN:H	1.70	0.55
3:H:145:HIS:CD2	3:H:164:ARG:HB3	2.43	0.54
2:D:25:ARG:NH1	2:D:71:ASP:OD2	2.39	0.54
2:B:106:GLU:OE2	2:B:174:TYR:OH	2.23	0.54
4:E:114:TYR:CD1	4:E:115:PRO:HA	2.44	0.53
2:D:68:SER:OG	6:D:301:HOH:O	2.18	0.53
3:F:106:ASN:HB3	3:F:146:LEU:HD13	1.90	0.52
3:H:275:ARG:O	3:H:278:ILE:HG12	2.09	0.52
3:H:266:ILE:O	3:H:270:GLN:HG3	2.10	0.52
3:H:278:ILE:HA	3:H:281:ILE:HD11	1.92	0.51
4:G:68:ASP:N	4:G:68:ASP:OD1	2.42	0.51
3:H:274:LEU:O	3:H:278:ILE:HG23	2.11	0.50
4:E:23:ALA:HA	4:E:51:ARG:HH12	1.76	0.50
4:G:15:THR:O	4:G:17:ARG:HG2	2.12	0.50
3:F:294:PHE:CD1	3:F:300:ILE:HG12	2.47	0.50
2:D:38:GLN:HB2	2:D:48:LEU:HD11	1.94	0.50
3:F:169:ARG:NH1	3:F:240:TYR:OH	2.46	0.49
3:H:161:ILE:HG13	3:H:192:LEU:HD21	1.94	0.49
4:G:114:TYR:CD1	4:G:115:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:194:ASN:HB3	3:H:261:LEU:HD23	1.95	0.49
4:E:99:GLU:HA	4:E:102:GLU:OE1	2.12	0.49
3:F:257:ARG:HB2	3:F:257:ARG:HH11	1.78	0.48
2:B:106:GLU:HG2	2:B:107:ILE:N	2.27	0.48
3:F:114:MET:O	3:F:118:THR:HG23	2.13	0.48
3:H:290:GLY:HA3	4:G:47:TYR:O	2.14	0.47
2:B:130:THR:OG1	6:B:301:HOH:O	2.19	0.47
3:H:281:ILE:HD13	4:G:58:TYR:CE2	2.48	0.47
3:H:233:ASP:O	3:H:236:ILE:HG12	2.15	0.47
1:C:121:LEU:HD21	6:C:325:HOH:O	2.15	0.47
3:H:264:GLY:O	3:H:268:LEU:HD13	2.15	0.47
3:H:165:PRO:HB3	3:H:206:ILE:HD11	1.97	0.47
2:B:25:ARG:N	6:B:302:HOH:O	2.25	0.47
1:C:15:VAL:HG11	1:C:89:LEU:HD13	1.97	0.47
1:C:63:TYR:HB2	1:C:68:LYS:HG3	1.97	0.47
3:F:290:GLY:HA3	4:E:47:TYR:O	2.16	0.46
4:G:114:TYR:CG	4:G:115:PRO:HA	2.51	0.46
4:G:4:LYS:HA	4:G:15:THR:CG2	2.45	0.46
3:H:121:LYS:HE2	3:H:122:ASN:OD1	2.16	0.46
3:F:258:ILE:HD11	3:F:266:ILE:HD13	1.98	0.46
4:E:23:ALA:HA	4:E:51:ARG:NH1	2.31	0.46
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.98	0.45
2:D:121:PRO:HD3	2:D:133:VAL:HG22	1.98	0.45
3:H:110:THR:HG23	3:H:113:ASN:H	1.82	0.45
3:F:167:ASP:OD1	3:F:204:SER:HB2	2.16	0.45
3:H:230:ILE:HG13	3:H:249:LEU:HD22	1.97	0.45
3:H:288:ARG:HD3	3:H:309:PRO:HG2	1.99	0.45
3:H:311:LEU:C	3:H:313:GLU:H	2.19	0.45
3:H:234:LYS:HE3	3:H:234:LYS:HB3	1.72	0.45
4:G:105:LEU:C	4:G:106:LYS:HD3	2.37	0.45
3:F:294:PHE:CZ	3:F:303:ILE:HD13	2.52	0.45
1:A:135:PHE:CE2	2:B:125:GLN:HG3	2.53	0.44
3:H:164:ARG:O	3:H:164:ARG:HG3	2.17	0.44
3:H:288:ARG:NE	3:H:309:PRO:HG3	2.33	0.44
2:D:106:GLU:HG2	2:D:107:ILE:N	2.33	0.44
3:F:258:ILE:CD1	3:F:266:ILE:HD13	2.48	0.44
3:H:309:PRO:HG2	4:G:52:ILE:HD13	1.99	0.44
2:D:108:LYS:HB3	2:D:108:LYS:HE2	1.73	0.44
3:H:110:THR:HG22	3:H:113:ASN:HB2	1.99	0.44
3:H:161:ILE:HG23	3:H:174:ILE:HG23	2.00	0.44
4:G:105:LEU:HA	4:G:109:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:123:ILE:HD12	3:F:157:VAL:HG12	2.00	0.43
3:H:237:TRP:CE3	3:H:241:ILE:HD11	2.53	0.43
4:G:56:ASN:CG	4:G:57:SER:H	2.12	0.43
3:F:283:LYS:O	3:F:286:ILE:HG22	2.19	0.43
4:G:56:ASN:HB2	4:G:68:ASP:HA	2.00	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.87	0.43
3:H:281:ILE:O	3:H:283:LYS:NZ	2.33	0.43
2:B:134:VAL:HG22	2:B:179:THR:HG23	2.01	0.42
4:G:71:LEU:CG	4:G:72:GLN:H	2.32	0.42
3:F:121:LYS:O	3:F:125:GLN:HG3	2.19	0.42
4:G:18:VAL:HG23	4:G:55:THR:CB	2.49	0.42
2:B:181:THR:HB	2:D:25:ARG:NH2	2.34	0.42
3:F:299:ASN:ND2	6:F:406:HOH:O	2.38	0.42
4:G:4:LYS:HA	4:G:15:THR:HG21	2.02	0.42
3:H:288:ARG:CZ	3:H:309:PRO:HG3	2.49	0.42
3:F:276:ARG:O	3:F:280:THR:HG23	2.20	0.42
3:H:201:ARG:HD2	3:H:254:MET:SD	2.60	0.42
3:F:101:GLU:HG2	3:F:151:ILE:HB	2.02	0.41
4:G:4:LYS:HB2	4:G:4:LYS:HE3	1.88	0.41
3:F:303:ILE:HG23	3:F:306:MET:HG2	2.02	0.41
2:B:126:LEU:O	2:B:184:LYS:HD3	2.19	0.41
3:H:133:LYS:HD3	3:H:133:LYS:N	2.36	0.41
3:H:133:LYS:HB2	3:H:134:GLU:H	1.63	0.41
1:A:108:GLU:HG3	3:H:257:ARG:HG2	2.03	0.41
1:A:225:GLU:HA	1:A:226:PRO:HD3	1.96	0.41
3:F:220:TYR:O	3:F:224:GLN:HG2	2.20	0.41
4:E:75:LYS:HD3	4:E:75:LYS:HA	1.86	0.40
3:F:295:LYS:HD3	3:F:295:LYS:HA	1.93	0.40
1:A:166:SER:OG	1:A:210:ASN:HB2	2.22	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	218/234 (93%)	204 (94%)	10 (5%)	4 (2%)	8	1
1	C	216/234 (92%)	212 (98%)	4 (2%)	0	100	100
2	B	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
2	D	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
3	F	189/254 (74%)	180 (95%)	7 (4%)	2 (1%)	14	5
3	H	177/254 (70%)	160 (90%)	12 (7%)	5 (3%)	5	1
4	E	118/122 (97%)	112 (95%)	6 (5%)	0	100	100
4	G	84/122 (69%)	76 (90%)	7 (8%)	1 (1%)	13	4
All	All	1424/1650 (86%)	1350 (95%)	62 (4%)	12 (1%)	19	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	305	PRO
3	H	234	LYS
3	H	307	THR
1	A	143	SER
1	A	172	LEU
3	F	309	PRO
3	H	309	PRO
1	A	226	PRO
1	A	140	SER
3	H	312	LYS
4	G	56	ASN
3	H	308	ILE

### 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	180/195 (92%)	176 (98%)	4 (2%)	52	46
1	C	182/195 (93%)	180 (99%)	2 (1%)	73	70
2	B	180/188 (96%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	184/188 (98%)	183 (100%)	1 (0%)	88	87
3	F	154/225 (68%)	154 (100%)	0	100	100
3	H	140/225 (62%)	138 (99%)	2 (1%)	67	62
4	E	101/106 (95%)	100 (99%)	1 (1%)	76	73
4	G	68/106 (64%)	60 (88%)	8 (12%)	5	1
All	All	1189/1428 (83%)	1171 (98%)	18 (2%)	65	59

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	78	SER
1	A	141	SER
1	A	201	SER
1	C	55	TYR
1	C	78	SER
2	D	106	GLU
4	E	102	GLU
3	H	276	ARG
3	H	277	LYS
4	G	15	THR
4	G	58	TYR
4	G	60	ILE
4	G	68	ASP
4	G	73	LEU
4	G	74	ILE
4	G	82	LEU
4	G	100	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	72	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](#)

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 4 ligands modelled in this entry, 4 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	222/234 (94%)	0.17	1 (0%) 91 91	36, 50, 87, 151	0
1	C	220/234 (94%)	0.27	1 (0%) 91 91	32, 44, 73, 150	0
2	B	213/215 (99%)	0.24	2 (0%) 84 85	35, 47, 83, 113	0
2	D	213/215 (99%)	0.27	3 (1%) 75 77	32, 43, 79, 115	0
3	F	199/254 (78%)	0.61	17 (8%) 10 12	43, 77, 127, 167	0
3	H	191/254 (75%)	0.84	23 (12%) 4 5	45, 84, 130, 161	0
4	E	120/122 (98%)	0.48	6 (5%) 28 31	51, 70, 102, 128	0
4	G	92/122 (75%)	0.88	13 (14%) 2 2	48, 85, 140, 190	0
All	All	1470/1650 (89%)	0.43	66 (4%) 33 35	32, 57, 112, 190	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	108	TYR	5.1
4	G	55	THR	5.0
4	G	61	LEU	4.9
1	C	228	SER	4.4
1	A	144	THR	4.1
3	H	273	ALA	4.1
4	G	58	TYR	4.1
3	F	309	PRO	4.0
2	D	28	GLN	4.0
3	H	308	ILE	3.8
3	H	120	LEU	3.7
3	H	276	ARG	3.6
4	G	71	LEU	3.6
3	H	239	GLY	3.6
3	F	308	ILE	3.6
4	G	104	TYR	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	H	178	ALA	3.5
3	H	307	THR	3.5
4	G	85	TRP	3.4
3	F	120	LEU	3.4
4	G	70	GLU	3.4
4	E	12	ALA	3.4
3	H	269	LEU	3.4
3	F	314	ALA	3.3
4	E	13	ASP	3.3
3	H	274	LEU	3.3
3	H	212	TYR	3.2
3	F	286	ILE	3.2
4	G	60	ILE	3.2
2	B	30	VAL	3.1
3	F	179	ILE	3.1
3	H	268	LEU	2.9
2	D	30	VAL	2.8
3	H	279	ARG	2.8
3	F	98	GLY	2.8
3	H	117	LEU	2.8
4	G	67	ALA	2.8
3	H	314	ALA	2.7
4	E	14	CYS	2.7
3	H	316	TRP	2.7
4	G	73	LEU	2.7
3	H	108	ASP	2.6
4	G	59	PRO	2.6
4	E	9	VAL	2.6
2	D	27	SER	2.5
3	F	122	ASN	2.4
4	E	62	CYS	2.4
3	F	303	ILE	2.4
3	H	128	LEU	2.3
3	F	137	ALA	2.3
3	H	272	ALA	2.3
3	H	229	GLU	2.3
3	H	102	PHE	2.2
3	F	292	GLU	2.2
3	F	294	PHE	2.2
3	F	176	PHE	2.2
4	E	26	PRO	2.1
3	F	218	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	256	PRO	2.1
3	F	239	GLY	2.1
3	H	311	LEU	2.1
3	F	240	TYR	2.1
3	H	124	PHE	2.1
4	G	107	TYR	2.0
2	B	31	SER	2.0
3	F	242	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. 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
5	ZN	G	202	1/1	0.72	0.39	124,124,124,124	0
5	ZN	G	201	1/1	0.89	0.19	96,96,96,96	0
5	ZN	E	201	1/1	0.91	0.23	107,107,107,107	0
5	ZN	E	202	1/1	0.99	0.05	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.