



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:40 PM UTC

PDB ID : 6CW3 / pdb_00006cw3
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

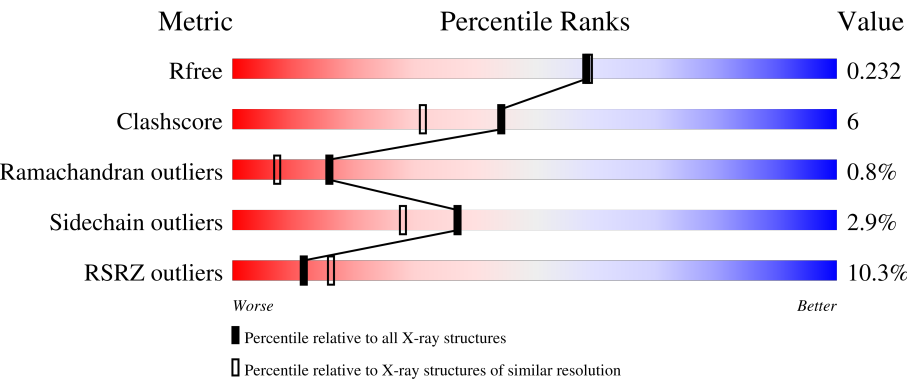
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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.



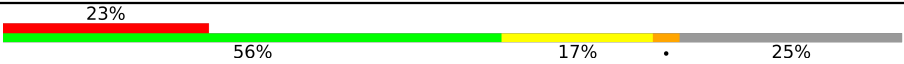
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	2% 88% 6% 5%
1	C	234	% 90% % 6%
2	B	215	4% 91% 7% ..
2	D	215	2% 90% 7% ..
3	F	254	16% 60% 17% 22%

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Mol	Chain	Length	Quality of chain
3	H	254	
4	E	122	
4	G	122	

2 Entry composition

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
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
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
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
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 (CCD ID: ZN) (formula: Zn).

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

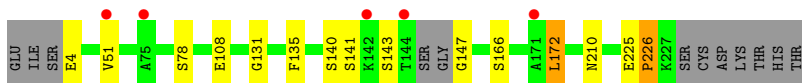
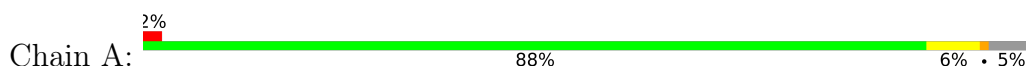
- Molecule 6 is water.

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

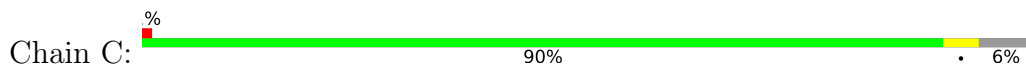
3 Residue-property plots [i](#)

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 heavy chain



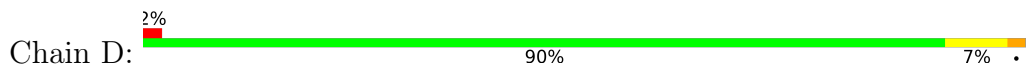
- Molecule 1: antibody heavy chain



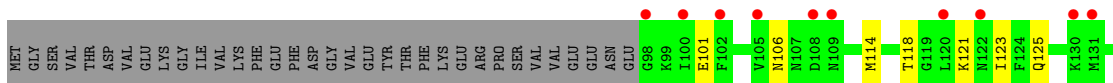
- Molecule 2: antibody light chain

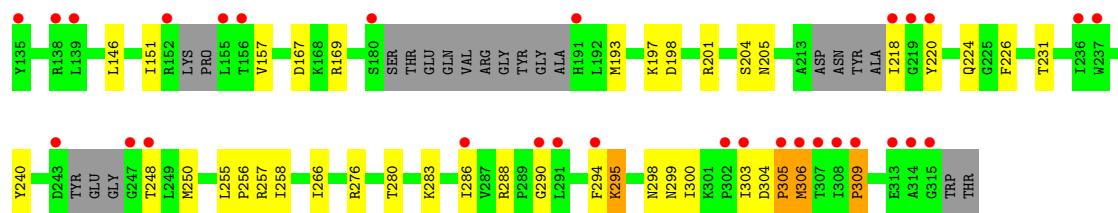


- Molecule 2: antibody light chain

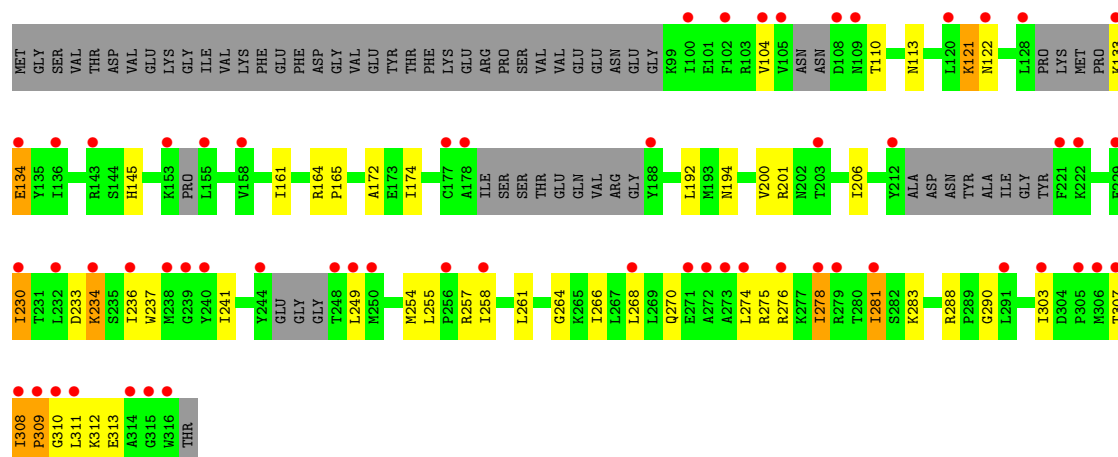


- Molecule 3: Histone acetyltransferase GCN5

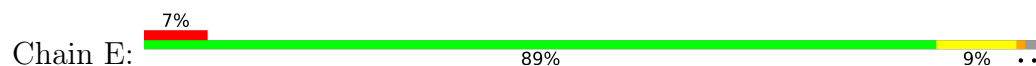




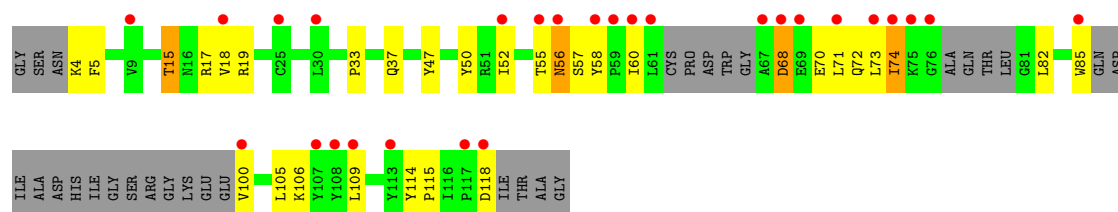
• Molecule 3: Histone acetyltransferase GCN5



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.203 , 0.227 0.208 , 0.232	Depositor DCC
R_{free} test set	6047 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11837	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.49	0/1708	0.81	2/2332 (0.1%)
1	C	0.58	0/1707	0.82	0/2326
2	B	0.53	0/1647	0.78	0/2238
2	D	0.55	0/1654	0.82	0/2247
3	F	0.44	0/1561	0.84	3/2104 (0.1%)
3	H	0.42	0/1469	0.93	5/1983 (0.3%)
4	E	0.43	0/966	0.74	0/1315
4	G	0.48	0/708	0.88	0/965
All	All	0.50	0/11420	0.83	10/15510 (0.1%)

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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	255	LEU	CA-C-N	6.13	127.50	119.84
3	H	255	LEU	C-N-CA	6.13	127.50	119.84
3	H	310	GLY	N-CA-C	-5.94	105.60	112.73
3	F	306	MET	N-CA-C	-5.77	104.91	112.41
3	H	134	GLU	N-CA-C	-5.63	106.40	113.72
1	A	131	GLY	CA-C-N	5.13	125.03	119.85
1	A	131	GLY	C-N-CA	5.13	125.03	119.85
3	F	255	LEU	CA-C-N	5.11	124.73	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	255	LEU	C-N-CA	5.11	124.73	119.05
3	H	230	ILE	N-CA-C	5.03	114.52	107.37

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 ⓘ

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	6	0
1	C	1662	0	1596	7	0
2	B	1613	0	1559	12	0
2	D	1620	0	1574	14	0
3	F	1535	0	1513	38	0
3	H	1448	0	1386	34	0
4	E	940	0	868	8	0
4	G	690	0	601	27	0
5	E	2	0	0	0	0
5	G	2	0	0	0	0
6	A	119	0	0	1	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	132	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 6.

All (132) 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
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
3:F:193:MET:HE2	3:F:226:PHE:HE1	1.63	0.62
3:H:308:ILE:HB	3:H:309:PRO:HD3	1.81	0.62
4:G:5:PHE:H	4:G:15:THR:HG23	1.65	0.62
3:F:288:ARG:HG3	3:F:309:PRO:HG3	1.80	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
1:C:92:GLU:HB2	2:D:5:MET:HE3	1.85	0.58
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:OD2	2:D:2:ASP:N	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
3:F:193:MET:HE3	3:F:197:LYS:HE3	1.88	0.55
4:G:71:LEU:HG	4:G:72:GLN:H	1.70	0.55
4:G:85:TRP:H	4:G:85:TRP:CD1	2.25	0.54
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
3:F:304:ASP:HB3	3:F:306:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:311:LEU:C	3:H:313:GLU:H	2.19	0.50
2:D:38:GLN:HB2	2:D:48:LEU:HD11	1.94	0.50
4:G:105:LEU:C	4:G:106:LYS:HD3	2.37	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
3:H:194:ASN:HB3	3:H:261:LEU:HD23	1.95	0.49
4:G:114:TYR:CD1	4:G:115:PRO:HA	2.48	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
4:G:56:ASN:CG	4:G:57:SER:H	2.12	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:233:ASP:O	3:H:236:ILE:HG12	2.15	0.47
3:H:281:ILE:HD13	4:G:58:TYR:CE2	2.48	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
3:H:121:LYS:HE2	3:H:122:ASN:OD1	2.16	0.46
4:G:4:LYS:HA	4:G:15:THR:CG2	2.45	0.46
4:G:114:TYR:CG	4:G:115:PRO:HA	2.51	0.46
3:F:193:MET:HE2	3:F:226:PHE:CE1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:288:ARG:HD3	3:H:309:PRO:HG2	1.99	0.45
3:H:234:LYS:HB3	3:H:234:LYS:HE3	1.72	0.45
2:B:48:LEU:C	2:B:49:ILE:HD12	2.42	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
1:C:109:MET:HE2	3:F:201:ARG:HB2	1.99	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:HE2	2:D:108:LYS:HB3	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
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
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:HD12	1:A:172:LEU:HA	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
1:C:109:MET:HE1	3:F:198:ASP:O	2.19	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:226:PHE:HB3	3:F:250:MET:HE2	2.01	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:N	3:H:133:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:220:TYR:O	3:F:224:GLN:HG2	2.20	0.41
3:F:304:ASP:OD1	3:F:304:ASP:C	2.64	0.41
1:C:23:LEU:HG	1:C:86:MET:HE2	2.03	0.40
3:F:197:LYS:NZ	3:F:224:GLN:O	2.50	0.40
3:F:295:LYS:HD3	3:F:295:LYS:HA	1.93	0.40
4:E:75:LYS:HD3	4:E:75:LYS:HA	1.86	0.40
4:G:118:ASP:C	4:G:118:ASP:OD1	2.64	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/234 (93%)	204 (94%)	10 (5%)	4 (2%)	6	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%)	11	4
3	H	177/254 (70%)	160 (90%)	12 (7%)	5 (3%)	4	0
4	E	118/122 (97%)	112 (95%)	6 (5%)	0	100	100
4	G	84/122 (69%)	76 (90%)	7 (8%)	1 (1%)	10	3
All	All	1424/1650 (86%)	1350 (95%)	62 (4%)	12 (1%)	16	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	305	PRO
3	H	234	LYS

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Mol	Chain	Res	Type
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%)	45	38
1	C	182/195 (93%)	180 (99%)	2 (1%)	65	61
2	B	180/188 (96%)	176 (98%)	4 (2%)	45	38
2	D	184/188 (98%)	177 (96%)	7 (4%)	29	19
3	F	154/225 (68%)	153 (99%)	1 (1%)	78	76
3	H	140/225 (62%)	133 (95%)	7 (5%)	22	10
4	E	101/106 (95%)	99 (98%)	2 (2%)	48	42
4	G	68/106 (64%)	61 (90%)	7 (10%)	7	1
All	All	1189/1428 (83%)	1155 (97%)	34 (3%)	37	28

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	51	VAL
1	A	78	SER
1	A	141	SER
2	B	3	ILE

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Mol	Chain	Res	Type
2	B	106	GLU
2	B	127	LYS
2	B	130	THR
1	C	68	LYS
1	C	78	SER
2	D	2	ASP
2	D	5	MET
2	D	30	VAL
2	D	82	GLU
2	D	106	GLU
2	D	146	LYS
2	D	170	LYS
3	F	295	LYS
4	E	102	GLU
4	E	119	ILE
3	H	121	LYS
3	H	200	VAL
3	H	258	ILE
3	H	276	ARG
3	H	278	ILE
3	H	281	ILE
3	H	303	ILE
4	G	15	THR
4	G	60	ILE
4	G	68	ASP
4	G	73	LEU
4	G	74	ILE
4	G	82	LEU
4	G	100	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
2	B	39	GLN
2	B	148	GLN
2	B	161	GLN
1	C	42	GLN
2	D	28	GLN
2	D	39	GLN
2	D	148	GLN
2	D	190	HIS

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Mol	Chain	Res	Type
3	F	122	ASN
4	E	72	GLN
4	E	91	HIS
3	H	125	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 oligosaccharides 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, 95th 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 ²)	Q < 0.9
1	A	222/234 (94%)	0.39	5 (2%) 61 70	36, 50, 87, 151	0
1	C	220/234 (94%)	0.17	2 (0%) 81 86	32, 44, 73, 150	0
2	B	213/215 (99%)	0.20	8 (3%) 44 54	35, 47, 83, 113	0
2	D	213/215 (99%)	0.12	4 (1%) 66 75	32, 43, 79, 115	0
3	F	199/254 (78%)	1.31	40 (20%) 3 3	43, 77, 127, 167	0
3	H	191/254 (75%)	1.61	58 (30%) 1 1	45, 84, 130, 161	0
4	E	120/122 (98%)	0.92	8 (6%) 24 31	51, 70, 102, 128	0
4	G	92/122 (75%)	1.67	27 (29%) 1 1	48, 85, 140, 190	0
All	All	1470/1650 (89%)	0.70	152 (10%) 12 16	32, 57, 112, 190	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	71	LEU	6.8
4	G	108	TYR	6.6
3	F	314	ALA	5.3
3	H	128	LEU	5.2
3	H	244	TYR	5.0
3	H	308	ILE	5.0
3	F	308	ILE	5.0
3	H	307	THR	4.8
3	H	221	PHE	4.8
3	F	315	GLY	4.8
2	B	30	VAL	4.7
1	A	144	THR	4.5
3	F	191	HIS	4.4
4	G	100	VAL	4.4
3	H	248	THR	4.4
4	G	55	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	H	314	ALA	4.3
3	H	188	TYR	4.3
3	F	309	PRO	4.1
3	H	273	ALA	4.1
4	G	75	LYS	4.0
3	F	294	PHE	4.0
3	F	155	LEU	4.0
3	H	316	TRP	3.9
4	G	73	LEU	3.9
3	F	286	ILE	3.9
4	E	120	THR	3.8
3	H	178	ALA	3.8
3	H	276	ARG	3.8
4	G	76	GLY	3.8
3	F	131	MET	3.8
3	H	133	LYS	3.8
4	G	61	LEU	3.7
3	H	278	ILE	3.7
3	F	219	GLY	3.6
3	F	108	ASP	3.6
4	G	74	ILE	3.5
3	H	108	ASP	3.5
3	F	100	ILE	3.5
4	G	67	ALA	3.5
2	D	28	GLN	3.4
2	B	31	SER	3.4
3	H	311	LEU	3.4
3	H	236	ILE	3.3
4	E	16	ASN	3.3
3	H	315	GLY	3.3
3	H	136	ILE	3.3
3	H	256	PRO	3.3
3	F	247	GLY	3.3
3	F	218	ILE	3.2
3	H	212	TYR	3.2
3	H	274	LEU	3.2
3	F	109	ASN	3.2
3	H	291	LEU	3.2
4	G	107	TYR	3.2
4	G	59	PRO	3.2
3	F	306	MET	3.2
3	F	290	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	F	236	ILE	3.1
3	F	180	SER	3.1
4	G	58	TYR	3.1
4	G	69	GLU	3.1
4	G	85	TRP	3.1
3	H	268	LEU	3.0
4	G	60	ILE	3.0
3	H	232	LEU	3.0
3	H	310	GLY	3.0
4	G	117	PRO	2.9
4	G	25	CYS	2.9
3	H	281	ILE	2.9
3	F	305	PRO	2.9
3	H	306	MET	2.9
4	G	30	LEU	2.9
3	H	238	MET	2.8
3	H	239	GLY	2.8
3	H	203	THR	2.8
3	H	222	LYS	2.8
3	F	307	THR	2.8
3	H	105	VAL	2.8
3	H	102	PHE	2.7
3	F	303	ILE	2.7
3	H	250	MET	2.7
3	H	104	VAL	2.7
3	H	272	ALA	2.7
2	B	42	GLY	2.7
4	G	118	ASP	2.7
2	B	29	SER	2.7
3	H	309	PRO	2.6
4	G	9	VAL	2.6
3	F	139	LEU	2.6
3	H	153	LYS	2.6
3	H	120	LEU	2.5
2	D	27	SER	2.5
1	A	142	LYS	2.5
4	G	56	ASN	2.5
3	F	313	GLU	2.5
3	H	158	VAL	2.5
3	H	279	ARG	2.5
1	A	171	ALA	2.5
3	H	249	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	230	ILE	2.4
2	B	70	THR	2.4
3	H	305	PRO	2.4
1	C	229	CYS	2.4
3	F	135	TYR	2.4
1	A	75	ALA	2.4
3	F	122	ASN	2.4
2	B	28	GLN	2.3
3	H	229	GLU	2.3
3	F	120	LEU	2.3
3	H	155	LEU	2.3
3	H	234	LYS	2.3
3	H	143	ARG	2.3
1	C	204	THR	2.3
3	H	109	ASN	2.3
3	H	122	ASN	2.3
3	H	258	ILE	2.2
4	E	24	ILE	2.2
3	F	105	VAL	2.2
4	E	105	LEU	2.2
4	G	109	LEU	2.2
2	B	3	ILE	2.2
3	H	303	ILE	2.2
4	E	60	ILE	2.2
3	F	248	THR	2.2
4	G	68	ASP	2.2
3	F	237	TRP	2.2
3	H	134	GLU	2.2
3	F	156	THR	2.2
3	F	243	ASP	2.2
2	B	69	GLY	2.2
3	F	98	GLY	2.2
3	F	302	PRO	2.2
2	D	100	GLY	2.1
3	F	152	ARG	2.1
4	E	26	PRO	2.1
3	H	100	ILE	2.1
3	H	240	TYR	2.1
1	A	51	VAL	2.1
2	D	146	LYS	2.1
3	H	271	GLU	2.1
3	F	220	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
4	G	113	TYR	2.1
3	F	130	LYS	2.1
3	F	291	LEU	2.1
3	H	177	CYS	2.1
3	F	102	PHE	2.0
4	G	18	VAL	2.0
4	E	13	ASP	2.0
4	G	52	ILE	2.0
4	E	1	GLY	2.0
3	F	138	ARG	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
5	ZN	G	202	1/1	0.91	0.23	124,124,124,124	0
5	ZN	E	201	1/1	0.96	0.15	107,107,107,107	0
5	ZN	G	201	1/1	0.97	0.10	96,96,96,96	0
5	ZN	E	202	1/1	0.99	0.12	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.