



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:15 PM UTC

PDB ID : 6CW2 / pdb_00006cw2
Title : Crystal structure of a yeast SAGA transcriptional coactivator Ada2/Gcn5 HAT subcomplex, crystal form 1
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 : 2.67 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

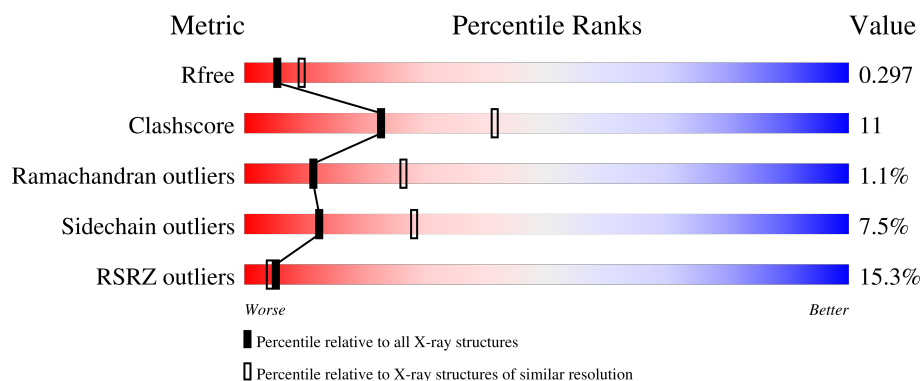
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	D	251	
2	C	120	
3	A	229	
4	B	215	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5948 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 Histone acetyltransferase GCN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	241	Total	C	N	O	S	0	0	0
			1872	1201	323	338	10			

- Molecule 2 is a protein called Transcriptional adapter 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	115	Total	C	N	O	S	0	0	0
			915	577	152	178	8			

- Molecule 3 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	217	Total	C	N	O	S	0	0	0
			1631	1047	266	310	8			

- Molecule 4 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	199	Total	C	N	O	S	0	0	0
			1477	925	245	301	6			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	12	Total	O	0	0
			12	12		

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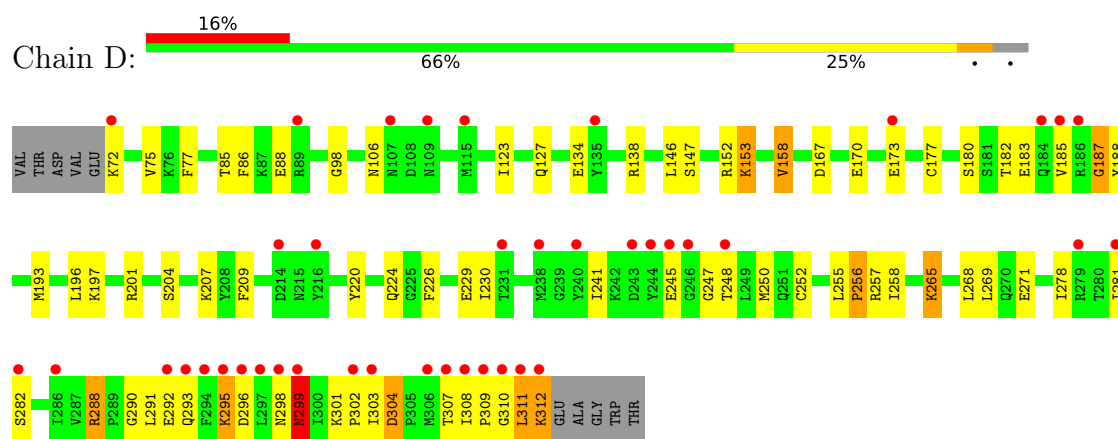
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	3	Total 3	O 3	0	0
6	A	12	Total 12	O 12	0	0
6	B	24	Total 24	O 24	0	0

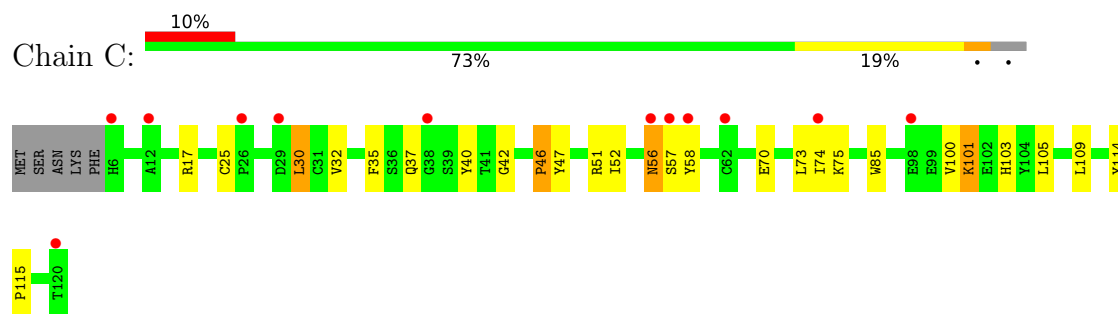
3 Residue-property plots [i](#)

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.

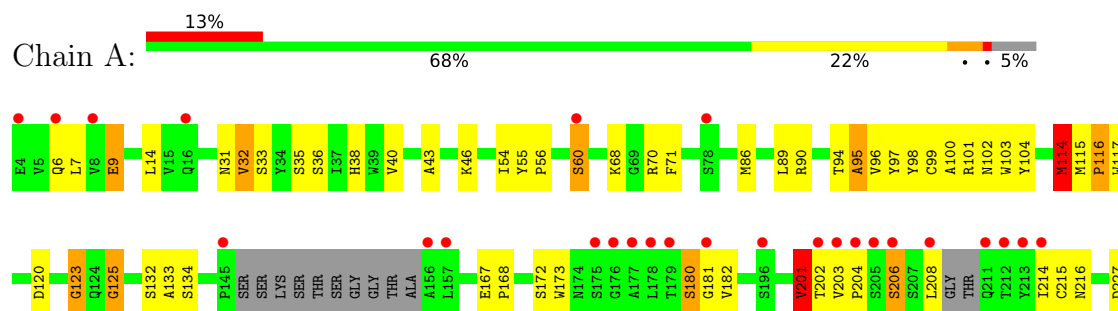
- Molecule 1: Histone acetyltransferase GCN5

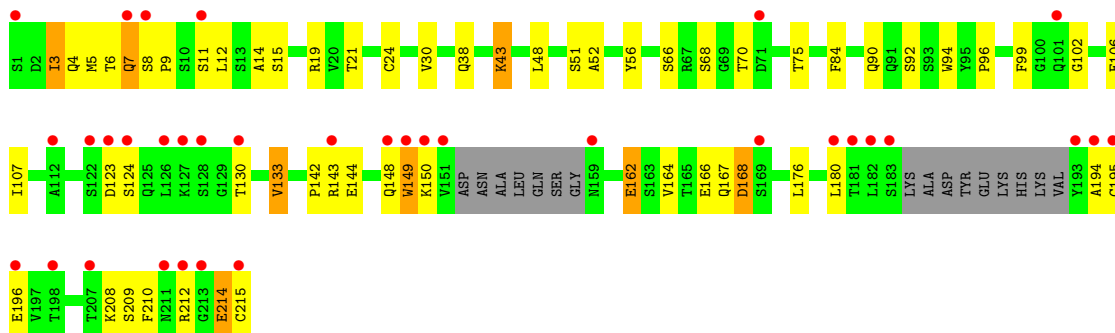


- Molecule 2: Transcriptional adapter 2



- Molecule 3: antibody heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.82Å 191.82Å 92.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.91 – 2.67 95.91 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.91-2.67) 99.8 (95.91-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.250 , 0.284 0.268 , 0.297	Depositor DCC
R_{free} test set	2713 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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	D	0.52	0/1909	1.15	14/2583 (0.5%)
2	C	0.52	0/940	1.01	2/1280 (0.2%)
3	A	0.59	0/1681	1.27	14/2300 (0.6%)
4	B	0.71	0/1509	1.36	19/2058 (0.9%)
All	All	0.59	0/6039	1.22	49/8221 (0.6%)

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
3	A	0	1
4	B	0	1
All	All	0	2

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	ILE	CA-C-N	-12.46	108.24	120.21
1	D	308	ILE	C-N-CA	-12.46	108.24	120.21
3	A	96	VAL	N-CA-C	-9.29	93.24	107.73
3	A	203	VAL	CA-C-N	8.83	128.56	119.56
3	A	203	VAL	C-N-CA	8.83	128.56	119.56
4	B	167	GLN	N-CA-C	8.60	122.63	110.50
2	C	25	CYS	CA-C-N	-8.53	110.94	119.90
2	C	25	CYS	C-N-CA	-8.53	110.94	119.90
1	D	187	GLY	N-CA-C	-8.52	100.79	115.61
4	B	166	GLU	N-CA-C	-8.45	99.37	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	GLN	CA-C-N	-8.22	111.19	122.86
4	B	4	GLN	C-N-CA	-8.22	111.19	122.86
3	A	123	GLY	N-CA-C	-8.16	100.12	112.60
3	A	201	VAL	N-CA-C	8.14	119.10	108.35
4	B	168	ASP	N-CA-C	7.96	121.95	110.10
4	B	99	PHE	CA-C-N	7.92	127.52	119.92
4	B	99	PHE	C-N-CA	7.92	127.52	119.92
3	A	6	GLN	N-CA-C	7.62	121.96	109.24
1	D	281	ILE	N-CA-C	-7.50	105.83	112.12
1	D	256	PRO	N-CA-C	6.88	122.62	113.40
4	B	6	THR	CA-C-N	-6.58	111.84	122.36
4	B	6	THR	C-N-CA	-6.58	111.84	122.36
3	A	60	SER	N-CA-C	6.48	120.85	109.96
4	B	148	GLN	N-CA-C	6.39	118.82	108.41
3	A	100	ALA	N-CA-C	6.30	119.53	108.75
4	B	162	GLU	N-CA-C	6.15	119.51	109.24
3	A	125	GLY	CA-C-N	5.90	130.51	122.19
3	A	125	GLY	C-N-CA	5.90	130.51	122.19
3	A	97	TYR	N-CA-C	5.87	118.24	109.25
3	A	6	GLN	CA-C-N	-5.86	114.54	122.86
3	A	6	GLN	C-N-CA	-5.86	114.54	122.86
1	D	310	GLY	N-CA-C	5.82	126.98	113.18
4	B	209	SER	N-CA-C	5.80	118.00	109.24
1	D	281	ILE	CA-C-N	5.77	128.91	120.71
1	D	281	ILE	C-N-CA	5.77	128.91	120.71
1	D	229	GLU	N-CA-C	5.77	117.46	109.15
4	B	149	TRP	N-CA-C	5.77	118.77	109.83
4	B	70	THR	CA-C-N	-5.71	110.59	122.07
4	B	70	THR	C-N-CA	-5.71	110.59	122.07
3	A	114	MET	N-CA-C	5.60	121.00	113.72
4	B	43	LYS	N-CA-C	5.59	117.51	110.24
1	D	308	ILE	N-CA-C	5.57	120.92	108.88
1	D	230	ILE	N-CA-C	5.30	114.85	106.32
4	B	14	ALA	N-CA-C	5.28	118.03	108.69
1	D	204	SER	N-CA-C	5.28	116.30	108.60
4	B	3	ILE	N-CA-C	5.24	114.81	107.37
1	D	298	ASN	N-CA-C	5.12	117.42	110.35
4	B	21	THR	N-CA-C	5.06	116.65	108.41
1	D	299	ASN	N-CA-C	5.02	117.33	110.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	180	SER	Peptide
4	B	210	PHE	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	D	1872	0	1841	47	0
2	C	915	0	848	17	0
3	A	1631	0	1527	38	0
4	B	1477	0	1375	32	0
5	C	2	0	0	0	0
6	A	12	0	0	1	0
6	B	24	0	0	3	0
6	C	3	0	0	0	0
6	D	12	0	0	2	0
All	All	5948	0	5591	121	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 11.

All (121) 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)
4:B:149:TRP:HE1	4:B:196:GLU:H	1.16	0.94
3:A:9:GLU:OE2	3:A:99:CYS:N	2.04	0.91
1:D:288:ARG:HH11	1:D:288:ARG:HG2	1.41	0.84
4:B:7:GLN:OE1	4:B:102:GLY:N	2.11	0.80
1:D:295:LYS:NZ	1:D:296:ASP:H	1.80	0.79
3:A:172:SER:HB3	3:A:216:ASN:HB2	1.65	0.79
1:D:177:CYS:SG	6:D:411:HOH:O	2.42	0.78
4:B:149:TRP:NE1	4:B:195:CYS:HA	2.00	0.77
4:B:212:ARG:HG2	4:B:214:GLU:HG3	1.72	0.71
3:A:216:ASN:ND2	3:A:227:ASP:OD1	2.22	0.67
1:D:271:GLU:HB2	2:C:74:ILE:HD13	1.76	0.66
1:D:106:ASN:HB3	1:D:146:LEU:HD23	1.76	0.66
3:A:134:SER:OG	6:A:301:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ILE:HG13	2:C:114:TYR:OH	1.95	0.65
4:B:149:TRP:HE1	4:B:196:GLU:N	1.90	0.65
4:B:52:ALA:O	6:B:301:HOH:O	2.14	0.64
4:B:149:TRP:NE1	4:B:196:GLU:H	1.92	0.64
1:D:304:ASP:OD1	1:D:304:ASP:N	2.32	0.62
4:B:143:ARG:O	4:B:143:ARG:NH2	2.32	0.61
3:A:36:SER:HB3	3:A:102:ASN:HB3	1.82	0.60
1:D:185:VAL:HG12	1:D:187:GLY:H	1.67	0.60
3:A:31:ASN:HD22	3:A:32:VAL:N	2.00	0.59
4:B:123:ASP:OD2	4:B:124:SER:N	2.36	0.59
3:A:214:ILE:HG22	3:A:216:ASN:HD21	1.70	0.56
1:D:301:LYS:O	1:D:303:ILE:N	2.34	0.56
3:A:167:GLU:HB3	3:A:168:PRO:HA	1.88	0.56
1:D:123:ILE:HD13	1:D:180:SER:HB2	1.86	0.55
2:C:114:TYR:CD1	2:C:115:PRO:HA	2.42	0.55
3:A:31:ASN:ND2	3:A:33:SER:H	2.04	0.54
1:D:311:LEU:HD22	2:C:32:VAL:HG11	1.89	0.54
1:D:185:VAL:HG12	1:D:187:GLY:N	2.23	0.54
3:A:31:ASN:O	3:A:35:SER:OG	2.24	0.53
4:B:133:VAL:HG13	4:B:180:LEU:HB3	1.91	0.53
3:A:55:TYR:HB2	3:A:60:SER:HB2	1.90	0.53
3:A:214:ILE:HG22	3:A:216:ASN:ND2	2.24	0.53
1:D:98:GLY:O	1:D:153:LYS:NZ	2.32	0.53
4:B:5:MET:HE3	4:B:24:CYS:SG	2.48	0.53
3:A:14:LEU:HD21	3:A:133:ALA:O	2.10	0.52
4:B:9:PRO:HB2	4:B:11:SER:O	2.09	0.52
1:D:301:LYS:O	1:D:303:ILE:HG13	2.08	0.52
4:B:149:TRP:HE1	4:B:195:CYS:HA	1.71	0.51
1:D:209:PHE:HB2	1:D:252:CYS:HB3	1.93	0.51
1:D:288:ARG:HG2	1:D:288:ARG:NH1	2.14	0.51
2:C:40:TYR:CD2	2:C:46:PRO:HD3	2.46	0.50
3:A:9:GLU:OE1	3:A:125:GLY:N	2.40	0.50
1:D:173:GLU:HB2	1:D:241:ILE:HG22	1.93	0.50
3:A:117:TRP:CZ2	4:B:51:SER:OG	2.64	0.50
1:D:295:LYS:HZ3	1:D:296:ASP:H	1.55	0.50
3:A:204:PRO:C	3:A:206:SER:H	2.19	0.50
1:D:295:LYS:HZ2	1:D:295:LYS:HB3	1.76	0.50
1:D:278:ILE:O	1:D:282:SER:HB3	2.12	0.50
2:C:105:LEU:HD23	2:C:109:LEU:HD23	1.94	0.49
3:A:116:PRO:O	4:B:90:GLN:NE2	2.33	0.49
3:A:71:PHE:CZ	3:A:86:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:LYS:HZ2	1:D:296:ASP:H	1.56	0.49
1:D:256:PRO:HG2	2:C:109:LEU:HD21	1.94	0.49
1:D:226:PHE:HB3	1:D:250:MET:HE2	1.93	0.49
3:A:70:ARG:NE	3:A:90:ARG:HH21	2.10	0.49
1:D:312:LYS:HD2	2:C:17:ARG:HD2	1.95	0.49
2:C:85:TRP:NE1	2:C:101:LYS:HG3	2.27	0.49
4:B:38:GLN:HB2	4:B:48:LEU:HD11	1.95	0.48
4:B:19:ARG:NH1	4:B:75:THR:HG21	2.27	0.48
2:C:56:ASN:O	2:C:58:TYR:N	2.46	0.48
1:D:290:GLY:HA3	2:C:47:TYR:O	2.14	0.48
3:A:54:ILE:HG12	3:A:56:PRO:HD3	1.96	0.48
1:D:299:ASN:HB3	2:C:37:GLN:HA	1.95	0.48
3:A:173:TRP:CH2	3:A:215:CYS:HB2	2.49	0.48
4:B:68:SER:OG	6:B:302:HOH:O	2.20	0.48
2:C:73:LEU:HD13	2:C:100:VAL:HG13	1.95	0.48
1:D:152:ARG:NH2	1:D:188:TYR:OH	2.47	0.47
3:A:36:SER:OG	3:A:38:HIS:NE2	2.41	0.47
4:B:3:ILE:HD13	4:B:30:VAL:HG12	1.97	0.47
3:A:31:ASN:HD22	3:A:31:ASN:C	2.23	0.47
1:D:220:TYR:O	1:D:224:GLN:HG2	2.15	0.47
1:D:269:LEU:HD23	1:D:269:LEU:HA	1.72	0.46
1:D:288:ARG:NH1	1:D:288:ARG:CG	2.79	0.46
3:A:182:VAL:HG22	3:A:201:VAL:HG13	1.97	0.46
4:B:162:GLU:OE2	4:B:176:LEU:HD21	2.16	0.46
3:A:36:SER:HB2	3:A:104:TYR:OH	2.16	0.46
1:D:291:LEU:O	1:D:293:GLN:N	2.49	0.46
4:B:106:GLU:HG2	4:B:107:ILE:N	2.31	0.46
4:B:149:TRP:CE2	4:B:194:ALA:O	2.69	0.45
3:A:9:GLU:OE1	3:A:123:GLY:HA3	2.16	0.45
3:A:38:HIS:CE1	3:A:116:PRO:HD3	2.51	0.45
3:A:7:LEU:O	3:A:123:GLY:HA2	2.17	0.45
3:A:43:ALA:HB3	3:A:46:LYS:HD2	1.98	0.45
4:B:143:ARG:CZ	4:B:164:VAL:HG21	2.47	0.45
1:D:147:SER:OG	6:D:401:HOH:O	2.21	0.44
3:A:86:MET:HB3	3:A:89:LEU:HD21	1.99	0.44
2:C:70:GLU:CD	2:C:103:HIS:HE2	2.25	0.44
1:D:158:VAL:HG22	1:D:183:GLU:OE2	2.18	0.44
1:D:158:VAL:HG22	1:D:183:GLU:CD	2.43	0.44
1:D:193:MET:HE3	1:D:196:LEU:HB3	1.99	0.44
1:D:295:LYS:HD2	1:D:295:LYS:HA	1.82	0.44
3:A:32:VAL:O	3:A:35:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:PHE:CZ	1:D:265:LYS:HG2	2.53	0.43
2:C:74:ILE:HD12	2:C:75:LYS:N	2.33	0.43
1:D:75:VAL:HG22	1:D:86:PHE:O	2.18	0.43
1:D:255:LEU:HD23	1:D:255:LEU:HA	1.83	0.43
1:D:304:ASP:HB2	1:D:307:THR:OG1	2.18	0.43
1:D:201:ARG:HB3	3:A:114:MET:HE1	2.01	0.43
3:A:103:TRP:HB2	3:A:120:ASP:HB2	2.00	0.43
1:D:86:PHE:HE2	1:D:88:GLU:OE2	2.02	0.42
3:A:180:SER:HA	3:A:181:GLY:HA2	1.80	0.42
1:D:193:MET:HE2	1:D:197:LYS:HG3	2.01	0.42
3:A:94:THR:O	3:A:95:ALA:HB2	2.18	0.42
3:A:40:VAL:O	3:A:98:TYR:HB2	2.19	0.42
4:B:194:ALA:HB1	4:B:208:LYS:O	2.20	0.42
1:D:207:LYS:HG2	4:B:94:TRP:CE3	2.54	0.42
2:C:114:TYR:CG	2:C:115:PRO:HA	2.55	0.41
1:D:245:GLU:C	1:D:247:GLY:H	2.28	0.41
4:B:142:PRO:HB2	4:B:144:GLU:OE1	2.20	0.41
3:A:117:TRP:HZ2	4:B:51:SER:OG	2.03	0.41
4:B:208:LYS:HD2	4:B:208:LYS:HA	1.84	0.41
1:D:307:THR:O	1:D:309:PRO:HD2	2.20	0.41
3:A:120:ASP:OD1	4:B:56:TYR:CZ	2.73	0.41
4:B:90:GLN:NE2	4:B:92:SER:HB3	2.35	0.41
4:B:84:PHE:HB2	4:B:107:ILE:HD13	2.03	0.41
4:B:212:ARG:NH1	6:B:309:HOH:O	2.53	0.41
2:C:30:LEU:HD23	2:C:35:PHE:HD1	1.85	0.41
1:D:170:GLU:OE2	1:D:207:LYS:NZ	2.38	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	D	239/251 (95%)	222 (93%)	15 (6%)	2 (1%)	16	34
2	C	113/120 (94%)	105 (93%)	5 (4%)	3 (3%)	4	9
3	A	211/229 (92%)	194 (92%)	15 (7%)	2 (1%)	14	31
4	B	193/215 (90%)	179 (93%)	13 (7%)	1 (0%)	24	45
All	All	756/815 (93%)	700 (93%)	48 (6%)	8 (1%)	11	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	GLU
2	C	57	SER
2	C	56	ASN
1	D	302	PRO
3	A	95	ALA
3	A	116	PRO
4	B	214	GLU
2	C	42	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/223 (86%)	174 (90%)	19 (10%)	7	17
2	C	100/107 (94%)	95 (95%)	5 (5%)	22	45
3	A	173/189 (92%)	162 (94%)	11 (6%)	16	35
4	B	162/190 (85%)	150 (93%)	12 (7%)	13	28
All	All	628/709 (89%)	581 (92%)	47 (8%)	12	28

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	72	LYS
1	D	85	THR
1	D	127	GLN

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Mol	Chain	Res	Type
1	D	134	GLU
1	D	138	ARG
1	D	153	LYS
1	D	158	VAL
1	D	167	ASP
1	D	182	THR
1	D	248	THR
1	D	257	ARG
1	D	265	LYS
1	D	268	LEU
1	D	288	ARG
1	D	295	LYS
1	D	299	ASN
1	D	304	ASP
1	D	311	LEU
1	D	312	LYS
2	C	30	LEU
2	C	46	PRO
2	C	51	ARG
2	C	52	ILE
2	C	101	LYS
3	A	9	GLU
3	A	32	VAL
3	A	68	LYS
3	A	101	ARG
3	A	114	MET
3	A	115	MET
3	A	132	SER
3	A	201	VAL
3	A	202	THR
3	A	206	SER
3	A	208	LEU
4	B	7	GLN
4	B	8	SER
4	B	12	LEU
4	B	15	SER
4	B	43	LYS
4	B	66	SER
4	B	96	PRO
4	B	130	THR
4	B	133	VAL
4	B	150	LYS

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Mol	Chain	Res	Type
4	B	168	ASP
4	B	215	CYS

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

Mol	Chain	Res	Type
3	A	31	ASN
4	B	139	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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	D	241/251 (96%)	0.96	41 (17%) 4 3	60, 83, 120, 164	0
2	C	115/120 (95%)	0.81	12 (10%) 11 10	60, 85, 113, 142	0
3	A	217/229 (94%)	0.91	30 (13%) 6 5	53, 84, 127, 160	0
4	B	199/215 (92%)	1.09	35 (17%) 4 3	52, 80, 143, 203	0
All	All	772/815 (94%)	0.96	118 (15%) 5 4	52, 83, 132, 203	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	308	ILE	7.6
2	C	58	TYR	7.5
3	A	208	LEU	7.3
4	B	151	VAL	7.1
2	C	57	SER	6.9
4	B	149	TRP	6.7
4	B	193	TYR	6.6
3	A	211	GLN	6.4
1	D	185	VAL	6.4
1	D	244	TYR	6.1
4	B	212	ARG	5.9
3	A	156	ALA	5.8
4	B	195	CYS	5.4
4	B	150	LYS	5.3
1	D	72	LYS	5.0
1	D	294	PHE	4.8
2	C	26	PRO	4.8
3	A	230	VAL	4.8
3	A	145	PRO	4.4
4	B	148	GLN	4.4
1	D	311	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	307	THR	4.4
1	D	184	GLN	4.3
2	C	6	HIS	4.2
4	B	194	ALA	4.1
1	D	246	GLY	4.1
1	D	186	ARG	4.1
4	B	211	ASN	4.0
4	B	213	GLY	4.0
4	B	183	SER	3.9
3	A	212	THR	3.8
4	B	159	ASN	3.8
1	D	115	MET	3.8
1	D	298	ASN	3.8
1	D	309	PRO	3.8
4	B	101	GLN	3.7
1	D	303	ILE	3.7
1	D	245	GLU	3.7
3	A	204	PRO	3.7
1	D	295	LYS	3.6
4	B	143	ARG	3.6
3	A	203	VAL	3.6
4	B	196	GLU	3.6
3	A	16	GLN	3.4
1	D	297	LEU	3.4
1	D	243	ASP	3.3
4	B	123	ASP	3.3
1	D	135	TYR	3.3
3	A	202	THR	3.3
4	B	122	SER	3.3
3	A	206	SER	3.2
2	C	29	ASP	3.2
1	D	306	MET	3.2
4	B	198	THR	3.2
3	A	179	THR	3.2
3	A	231	GLU	3.1
3	A	176	GLY	3.1
1	D	286	ILE	3.0
4	B	126	LEU	3.0
2	C	120	THR	3.0
4	B	130	THR	3.0
4	B	207	THR	2.9
1	D	312	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	177	ALA	2.9
3	A	229	LYS	2.8
4	B	215	CYS	2.8
2	C	74	ILE	2.8
1	D	293	GLN	2.8
1	D	310	GLY	2.8
4	B	181	THR	2.7
3	A	232	PRO	2.7
4	B	128	SER	2.7
1	D	238	MET	2.7
3	A	205	SER	2.7
1	D	216	TYR	2.6
4	B	71	ASP	2.6
3	A	214	ILE	2.6
2	C	98	GLU	2.5
3	A	178	LEU	2.5
1	D	231	THR	2.5
2	C	62	CYS	2.5
1	D	302	PRO	2.5
1	D	299	ASN	2.4
3	A	175	SER	2.4
4	B	180	LEU	2.4
1	D	107	ASN	2.4
1	D	109	ASN	2.4
1	D	282	SER	2.4
4	B	127	LYS	2.4
3	A	4	GLU	2.3
3	A	213	TYR	2.3
2	C	12	ALA	2.3
3	A	60	SER	2.2
1	D	281	ILE	2.2
1	D	292	GLU	2.2
1	D	240	TYR	2.2
4	B	7	GLN	2.2
1	D	296	ASP	2.2
1	D	173	GLU	2.1
1	D	248	THR	2.1
3	A	157	LEU	2.1
4	B	182	LEU	2.1
3	A	8	VAL	2.1
4	B	1	SER	2.1
4	B	11	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	89	ARG	2.1
1	D	214	ASP	2.1
4	B	169	SER	2.1
2	C	56	ASN	2.1
3	A	181	GLY	2.1
3	A	78	SER	2.0
1	D	279	ARG	2.0
4	B	112	ALA	2.0
3	A	196	SER	2.0
4	B	8	SER	2.0
4	B	124	SER	2.0
3	A	6	GLN	2.0
2	C	38	GLY	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($\text{\AA}^2$)	Q<0.9
5	ZN	C	201	1/1	0.99	0.07	91,91,91,91	0
5	ZN	C	202	1/1	1.00	0.04	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.