



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 AM UTC

PDB ID : 3M99 / pdb_00003m99
Title : Structure of the Ubp8-Sgf11-Sgf73-Sus1 SAGA DUB module
Authors : Kohler, A.; Zimmerman, E.; Schneider, M.; Hurt, E.; Zheng, N.
Deposited on : 2010-03-21
Resolution : 2.70 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

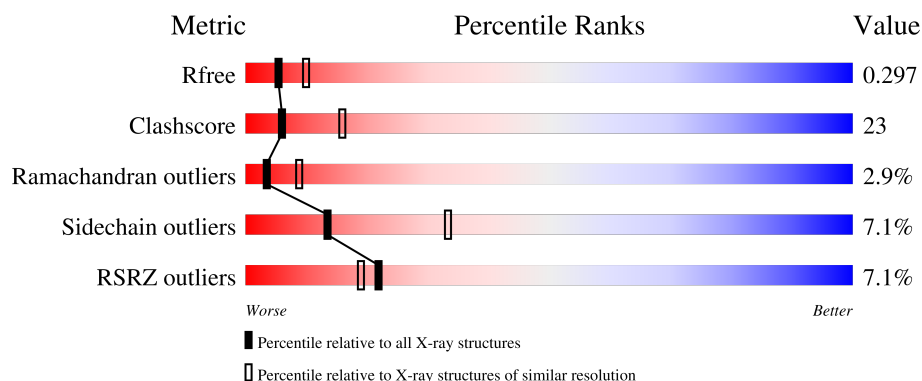
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

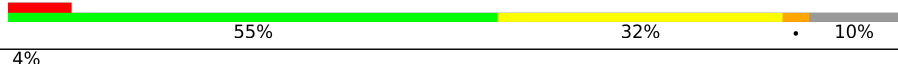
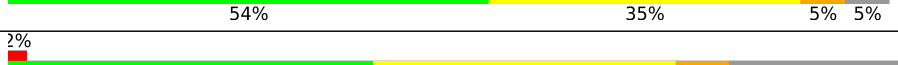
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	471	
2	B	99	
3	C	96	
4	D	104	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5557 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 Ubiquitin carboxyl-terminal hydrolase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3382	2154	575	620	33			

- Molecule 2 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			710	434	132	141	3			

- Molecule 3 is a protein called Protein SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			737	460	121	154	2			

- Molecule 4 is a protein called SAGA-associated factor 73.

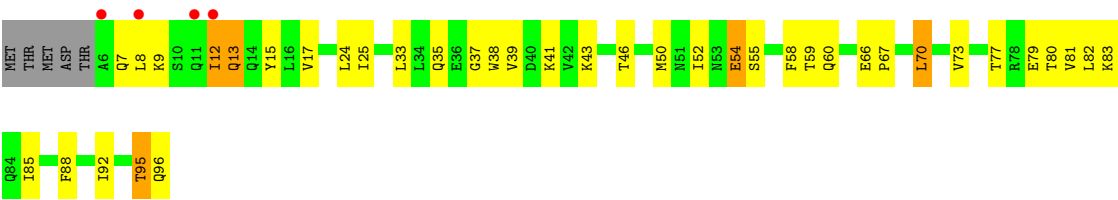
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	84	Total	C	N	O	S	0	0	0
			680	432	114	129	5			

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

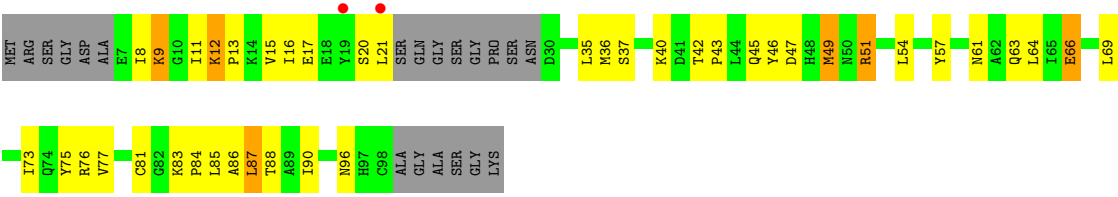
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	Zn	0	0
			5	5		
5	B	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	2	Total 2	O 2	0	0
6	C	2	Total 2	O 2	0	0
6	D	5	Total 5	O 5	0	0



● Molecule 4: SAGA-associated factor 73



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.42Å 103.52Å 70.35Å 90.00° 108.09° 90.00°	Depositor
Resolution (Å)	48.12 – 2.70 48.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.8 (48.12-2.70) 88.9 (48.12-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.234 , 0.300 0.230 , 0.297	Depositor DCC
R_{free} test set	1186 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.818	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5557	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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	0.39	0/3453	0.83	10/4647 (0.2%)
2	B	0.36	0/718	1.09	3/971 (0.3%)
3	C	0.37	0/743	0.77	0/1000
4	D	0.42	0/694	0.90	2/935 (0.2%)
All	All	0.39	0/5608	0.87	15/7553 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	GLU	CB-CA-C	-18.91	79.61	110.81
2	B	67	SER	N-CA-C	-8.82	92.01	110.80
1	A	158	ASN	CA-C-N	7.69	127.24	119.24
1	A	158	ASN	C-N-CA	7.69	127.24	119.24
1	A	368	LEU	N-CA-C	7.03	119.97	111.40
1	A	301	ASP	CA-C-N	6.74	126.65	119.85
1	A	301	ASP	C-N-CA	6.74	126.65	119.85
2	B	67	SER	N-CA-CB	-6.51	99.50	110.49
4	D	12	LYS	CA-C-N	6.12	126.01	119.28
4	D	12	LYS	C-N-CA	6.12	126.01	119.28
1	A	406	VAL	CA-C-N	5.55	126.40	120.13
1	A	406	VAL	C-N-CA	5.55	126.40	120.13
1	A	194	LEU	N-CA-C	-5.47	108.38	114.62
1	A	406	VAL	CB-CA-C	-5.10	101.70	111.40
1	A	245	ILE	CB-CA-C	-5.08	105.46	111.81

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	3382	0	3312	177	0
2	B	710	0	698	32	0
3	C	737	0	742	33	0
4	D	680	0	678	50	0
5	A	5	0	0	1	0
5	B	1	0	0	1	0
5	D	1	0	0	0	0
6	A	32	0	0	4	0
6	B	2	0	0	0	0
6	C	2	0	0	3	0
6	D	5	0	0	4	0
All	All	5557	0	5430	250	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 23.

All (250) 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:66:GLU:CG	2:B:66:GLU:O	1.80	1.19
4:D:37:SER:HA	6:D:110:HOH:O	1.51	1.09
1:A:364:ARG:HH22	1:A:459:GLN:HG3	1.23	1.03
2:B:66:GLU:O	2:B:66:GLU:HG3	1.21	1.00
1:A:43:THR:HB	1:A:59:MET:HE2	1.44	0.99
1:A:60:CYS:CB	1:A:63:CYS:SG	2.51	0.99
1:A:31:LEU:HD21	1:A:59:MET:HE1	1.48	0.96
4:D:51:ARG:HH11	4:D:51:ARG:HG2	1.36	0.88
1:A:156:ILE:O	1:A:162:ILE:HD11	1.74	0.87
1:A:274:ILE:HD12	1:A:274:ILE:H	1.39	0.87
2:B:57:ASP:HB2	2:B:61:LEU:H	1.39	0.87
2:B:76:CYS:SG	5:B:100:ZN:ZN	1.64	0.86
1:A:3:ILE:HD12	1:A:4:CYS:H	1.40	0.85
3:C:25:ILE:HD13	3:C:85:ILE:HD13	1.61	0.82
1:A:329:LEU:HB3	1:A:345:ALA:HB3	1.63	0.81
1:A:60:CYS:HB3	1:A:63:CYS:SG	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:LEU:O	6:C:98:HOH:O	1.99	0.81
1:A:406:VAL:HG13	4:D:57:TYR:OH	1.80	0.80
4:D:37:SER:CA	6:D:110:HOH:O	2.19	0.79
1:A:78:SER:HB2	1:A:83:HIS:O	1.83	0.78
2:B:16:LEU:HD22	3:C:82:LEU:HD13	1.65	0.77
1:A:364:ARG:NH2	1:A:459:GLN:HG3	1.98	0.77
4:D:37:SER:CB	6:D:110:HOH:O	2.33	0.77
1:A:4:CYS:HB3	1:A:7:ILE:HD11	1.68	0.76
1:A:54:SER:HB3	1:A:68:CYS:HB2	1.67	0.75
1:A:9:GLN:HA	1:A:12:GLN:HE21	1.49	0.75
2:B:8:ILE:HG12	4:D:8:ILE:HG13	1.67	0.75
1:A:310:ILE:HG23	1:A:380:ILE:HD11	1.66	0.75
1:A:357:VAL:HG22	1:A:466:THR:HG22	1.69	0.74
1:A:180:ASP:HB3	1:A:181:LYS:HD2	1.68	0.74
1:A:310:ILE:HD12	1:A:380:ILE:HD12	1.71	0.73
3:C:73:VAL:HG22	6:C:98:HOH:O	1.89	0.72
4:D:51:ARG:HH11	4:D:51:ARG:CG	2.03	0.72
1:A:246:ILE:HG23	1:A:275:VAL:HG11	1.71	0.71
1:A:237:ASP:HB3	1:A:240:GLU:CG	2.21	0.69
1:A:180:ASP:N	6:A:508:HOH:O	2.24	0.69
1:A:104:GLY:O	1:A:106:ILE:N	2.25	0.69
1:A:7:ILE:HG12	1:A:103:ILE:HD13	1.72	0.69
1:A:438:GLN:H	1:A:438:GLN:NE2	1.91	0.68
1:A:88:ASN:HB3	1:A:91:ASN:HD21	1.58	0.68
4:D:36:MET:HG3	4:D:40:LYS:HE2	1.76	0.68
2:B:30:ARG:O	2:B:34:GLN:HG3	1.93	0.68
1:A:88:ASN:HD22	1:A:91:ASN:CG	2.02	0.68
3:C:46:THR:HG22	3:C:50:MET:HE2	1.75	0.68
1:A:4:CYS:O	1:A:7:ILE:HD12	1.94	0.67
1:A:91:ASN:HD22	1:A:93:LEU:H	1.40	0.67
2:B:23:LEU:O	2:B:27:ILE:HG12	1.95	0.67
2:B:75:ASN:HD22	2:B:93:LEU:HD23	1.60	0.66
1:A:174:CYS:SG	5:A:475:ZN:ZN	1.84	0.66
1:A:310:ILE:HG23	1:A:380:ILE:CD1	2.26	0.65
1:A:368:LEU:HD13	1:A:374:ARG:HH11	1.61	0.64
1:A:3:ILE:HD12	1:A:4:CYS:N	2.11	0.64
2:B:75:ASN:ND2	2:B:93:LEU:HD23	2.13	0.63
1:A:88:ASN:HB3	1:A:91:ASN:ND2	2.13	0.63
3:C:25:ILE:HG21	3:C:85:ILE:HD11	1.81	0.62
1:A:129:SER:O	1:A:131:GLU:N	2.33	0.62
1:A:406:VAL:CG1	4:D:57:TYR:CZ	2.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:PRO:O	4:D:16:ILE:HG12	1.99	0.62
1:A:190:ILE:O	1:A:194:LEU:HB2	2.00	0.62
1:A:462:LEU:O	1:A:463:LEU:HD23	2.00	0.61
4:D:49:MET:HB3	4:D:54:LEU:HD11	1.82	0.61
1:A:90:ASN:HD21	2:B:22:THR:HG22	1.64	0.61
1:A:250:HIS:ND1	1:A:276:HIS:HE1	1.99	0.61
1:A:411:TYR:HB3	1:A:465:TYR:HB3	1.82	0.61
2:B:20:LEU:O	2:B:24:ILE:HG12	2.00	0.61
1:A:4:CYS:HB3	1:A:7:ILE:CD1	2.31	0.61
1:A:250:HIS:ND1	1:A:276:HIS:CE1	2.68	0.60
1:A:431:PHE:HE2	1:A:450:ILE:HD13	1.67	0.60
1:A:406:VAL:HG11	4:D:57:TYR:CZ	2.37	0.60
1:A:277:THR:CG2	4:D:63:GLN:HB2	2.32	0.59
1:A:274:ILE:HD12	1:A:274:ILE:N	2.13	0.58
1:A:368:LEU:HD12	1:A:374:ARG:HD2	1.85	0.58
1:A:58:PHE:O	1:A:66:CYS:HA	2.03	0.58
1:A:237:ASP:HB3	1:A:240:GLU:HG3	1.85	0.57
1:A:237:ASP:HB3	1:A:240:GLU:HG2	1.85	0.57
1:A:274:ILE:H	1:A:274:ILE:CD1	2.05	0.57
1:A:21:LEU:C	6:A:488:HOH:O	2.47	0.57
1:A:366:GLU:OE1	1:A:368:LEU:HD21	2.04	0.57
1:A:368:LEU:HD13	1:A:374:ARG:NH1	2.20	0.56
1:A:148:MET:HA	1:A:241:PHE:CD2	2.39	0.56
1:A:470:VAL:O	1:A:471:ASN:HB2	2.05	0.56
1:A:164:HIS:CG	1:A:274:ILE:HG12	2.39	0.56
1:A:241:PHE:O	1:A:245:ILE:HG12	2.06	0.56
1:A:366:GLU:HB2	1:A:368:LEU:HG	1.87	0.56
3:C:15:TYR:CD1	3:C:92:ILE:HD13	2.40	0.56
1:A:219:LEU:C	1:A:219:LEU:HD23	2.31	0.56
3:C:95:THR:HG23	3:C:96:GLN:H	1.70	0.56
3:C:33:LEU:HD22	3:C:38:TRP:CD2	2.41	0.55
1:A:48:THR:HG21	1:A:73:HIS:CD2	2.41	0.55
1:A:277:THR:HG22	4:D:63:GLN:H	1.72	0.55
3:C:92:ILE:HA	4:D:15:VAL:HG21	1.87	0.55
1:A:61:LEU:HD23	1:A:61:LEU:O	2.07	0.54
3:C:39:VAL:N	6:C:97:HOH:O	2.40	0.54
1:A:277:THR:HG22	4:D:63:GLN:HB2	1.88	0.54
1:A:130:MET:HE1	2:B:46:ARG:HG3	1.90	0.54
1:A:219:LEU:HD23	1:A:219:LEU:O	2.07	0.54
3:C:37:GLY:O	3:C:41:LYS:HB2	2.08	0.54
1:A:49:CYS:HB3	1:A:73:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HB3	1:A:194:LEU:HD11	1.90	0.53
1:A:192:HIS:HE1	1:A:197:ALA:O	1.90	0.53
2:B:79:ASP:OD2	2:B:79:ASP:N	2.41	0.53
3:C:7:GLN:C	3:C:9:LYS:H	2.16	0.53
1:A:44:MET:O	1:A:52:ILE:HA	2.09	0.53
1:A:375:LYS:HD2	1:A:375:LYS:O	2.09	0.53
1:A:320:LEU:HD13	1:A:388:MET:HE1	1.90	0.52
1:A:365:PHE:O	1:A:366:GLU:HG2	2.09	0.52
4:D:51:ARG:CG	4:D:51:ARG:NH1	2.69	0.52
1:A:24:CYS:SG	1:A:87:ILE:HD11	2.50	0.52
1:A:59:MET:HE3	1:A:89:SER:HA	1.90	0.52
2:B:11:ILE:O	2:B:15:ILE:HG12	2.09	0.52
3:C:50:MET:HG2	3:C:55:SER:O	2.09	0.52
2:B:27:ILE:HG23	3:C:43:LYS:HG2	1.92	0.52
3:C:66:GLU:O	3:C:70:LEU:HB2	2.09	0.52
1:A:277:THR:HG22	4:D:63:GLN:N	2.24	0.51
1:A:91:ASN:ND2	1:A:93:LEU:H	2.08	0.51
1:A:417:VAL:HB	1:A:462:LEU:HB2	1.92	0.51
4:D:86:ALA:C	4:D:88:THR:H	2.17	0.51
1:A:90:ASN:HD21	2:B:22:THR:CG2	2.23	0.51
1:A:115:ALA:O	1:A:116:LYS:HB2	2.09	0.51
1:A:192:HIS:CE1	1:A:198:LEU:HB2	2.46	0.51
1:A:413:LEU:HD21	1:A:416:ILE:HD11	1.92	0.51
1:A:285:SER:HB2	1:A:299:THR:OG1	2.11	0.51
1:A:429:ILE:HD12	1:A:443:ASN:HA	1.93	0.51
3:C:77:THR:O	3:C:81:VAL:HG23	2.10	0.51
4:D:49:MET:HE3	4:D:64:LEU:HD13	1.93	0.51
1:A:125:THR:HG23	4:D:76:ARG:HH21	1.75	0.50
3:C:39:VAL:O	3:C:43:LYS:HG3	2.10	0.50
1:A:6:HIS:O	1:A:10:VAL:HG23	2.12	0.50
1:A:211:ASN:O	1:A:213:GLN:N	2.44	0.50
1:A:192:HIS:ND1	1:A:192:HIS:C	2.68	0.50
1:A:237:ASP:OD2	1:A:240:GLU:HG2	2.11	0.50
1:A:322:SER:O	1:A:325:LYS:HG3	2.11	0.50
1:A:384:THR:HG23	1:A:385:TYR:CD1	2.47	0.50
1:A:52:ILE:HG12	3:C:13:GLN:OE1	2.12	0.49
2:B:49:TYR:HE2	2:B:51:ASP:HB2	1.75	0.49
1:A:387:ASN:HD22	3:C:35:GLN:HE22	1.59	0.49
1:A:418:SER:HB2	1:A:459:GLN:O	2.12	0.49
1:A:87:ILE:HG13	1:A:94:LEU:HD13	1.95	0.49
1:A:53:ASN:HA	6:A:505:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:HD13	1:A:445:SER:HB3	1.94	0.49
1:A:42:ASN:HB3	4:D:35:LEU:HD11	1.95	0.49
1:A:151:ILE:HD11	1:A:462:LEU:CD1	2.43	0.49
4:D:76:ARG:NH2	6:D:109:HOH:O	2.46	0.49
1:A:311:LYS:HD2	1:A:313:LYS:HE3	1.96	0.48
1:A:406:VAL:HG13	4:D:57:TYR:CZ	2.46	0.48
1:A:88:ASN:ND2	1:A:91:ASN:OD1	2.43	0.48
1:A:181:LYS:HD2	1:A:181:LYS:N	2.28	0.48
1:A:366:GLU:OE1	1:A:368:LEU:HD11	2.14	0.48
4:D:86:ALA:O	4:D:90:ILE:HG13	2.13	0.48
1:A:132:ARG:NE	1:A:132:ARG:HA	2.28	0.48
1:A:277:THR:HG23	4:D:61:ASN:O	2.14	0.48
1:A:382:PHE:CE1	1:A:460:ALA:HB2	2.48	0.48
2:B:84:ARG:HH12	2:B:91:ARG:HH21	1.61	0.48
3:C:96:GLN:HB3	4:D:9:LYS:HZ3	1.79	0.48
1:A:38:GLU:O	1:A:42:ASN:HB2	2.14	0.47
2:B:49:TYR:N	2:B:58:ILE:O	2.39	0.47
1:A:311:LYS:HB2	1:A:313:LYS:HE3	1.96	0.46
2:B:76:CYS:SG	2:B:88:HIS:NE2	2.88	0.46
1:A:102:TYR:HE2	3:C:58:PHE:CD1	2.33	0.46
1:A:406:VAL:CG1	4:D:57:TYR:OH	2.58	0.46
1:A:226:ILE:C	1:A:227:ASN:HD22	2.23	0.46
1:A:438:GLN:H	1:A:438:GLN:CD	2.23	0.46
4:D:75:TYR:HB2	4:D:85:LEU:O	2.15	0.46
1:A:24:CYS:N	6:A:488:HOH:O	2.48	0.46
1:A:288:VAL:HB	1:A:346:ILE:HG23	1.97	0.46
1:A:125:THR:CG2	4:D:76:ARG:HH21	2.28	0.46
3:C:66:GLU:HB3	3:C:67:PRO:HD3	1.98	0.46
1:A:166:MET:HE1	4:D:73:ILE:HD11	1.97	0.46
1:A:31:LEU:CD2	1:A:59:MET:HE1	2.33	0.45
1:A:53:ASN:O	2:B:18:ASN:HB3	2.16	0.45
1:A:56:ALA:HB1	1:A:88:ASN:OD1	2.16	0.45
3:C:79:GLU:O	3:C:83:LYS:HB2	2.17	0.45
1:A:311:LYS:C	1:A:313:LYS:H	2.24	0.45
1:A:121:VAL:O	1:A:125:THR:HG22	2.16	0.45
1:A:158:ASN:O	1:A:162:ILE:HG12	2.16	0.45
3:C:12:ILE:HD13	3:C:12:ILE:O	2.15	0.45
3:C:54:GLU:CD	3:C:54:GLU:C	2.84	0.45
1:A:8:GLN:O	1:A:12:GLN:HG3	2.17	0.45
1:A:86:GLY:O	1:A:94:LEU:HD12	2.16	0.45
1:A:148:MET:HB3	1:A:241:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HD13	1:A:5:PRO:HD3	1.98	0.45
1:A:49:CYS:O	1:A:50:HIS:HB2	2.17	0.45
1:A:166:MET:HE1	4:D:73:ILE:CG1	2.46	0.45
1:A:270:GLN:HA	1:A:270:GLN:OE1	2.17	0.45
4:D:81:CYS:SG	4:D:83:LYS:HB2	2.57	0.45
2:B:51:ASP:OD1	2:B:55:SER:HB3	2.16	0.45
2:B:70:TYR:CD1	2:B:79:ASP:HB3	2.52	0.45
1:A:71:HIS:HB2	1:A:73:HIS:CE1	2.52	0.45
1:A:81:ILE:O	1:A:81:ILE:HG22	2.17	0.45
4:D:64:LEU:HD23	4:D:64:LEU:HA	1.73	0.45
1:A:42:ASN:CB	4:D:35:LEU:HD11	2.47	0.44
1:A:246:ILE:HG23	1:A:275:VAL:CG1	2.42	0.44
1:A:368:LEU:HD12	1:A:374:ARG:CD	2.48	0.44
1:A:209:SER:OG	2:B:69:GLN:HG2	2.18	0.44
1:A:277:THR:HG22	4:D:63:GLN:CB	2.47	0.44
1:A:386:LEU:HD21	1:A:388:MET:HE3	1.99	0.44
3:C:7:GLN:O	3:C:7:GLN:HG2	2.18	0.44
1:A:31:LEU:HD21	1:A:59:MET:CE	2.33	0.44
1:A:282:SER:N	1:A:303:PHE:CE2	2.86	0.44
2:B:73:CYS:O	2:B:76:CYS:O	2.35	0.44
1:A:246:ILE:HG22	1:A:247:ASN:N	2.32	0.44
1:A:131:GLU:CD	2:B:46:ARG:HH21	2.25	0.44
4:D:46:TYR:HD2	4:D:66:GLU:HG2	1.83	0.43
1:A:71:HIS:HB2	1:A:73:HIS:ND1	2.33	0.43
1:A:245:ILE:O	1:A:246:ILE:C	2.61	0.43
2:B:8:ILE:HA	4:D:8:ILE:CD1	2.48	0.43
4:D:12:LYS:HB3	4:D:15:VAL:HG23	2.00	0.43
1:A:287:ILE:O	1:A:296:SER:HA	2.18	0.43
1:A:436:GLY:HA3	1:A:438:GLN:OE1	2.19	0.43
3:C:25:ILE:HD11	3:C:88:PHE:HD1	1.84	0.43
3:C:52:ILE:C	3:C:54:GLU:H	2.26	0.43
1:A:176:VAL:HG21	1:A:182:CYS:HB2	2.01	0.43
4:D:87:LEU:HD22	4:D:87:LEU:HA	1.90	0.43
1:A:388:MET:HE2	1:A:388:MET:HA	2.01	0.42
2:B:61:LEU:HA	2:B:61:LEU:HD23	1.81	0.42
1:A:121:VAL:O	1:A:125:THR:CG2	2.66	0.42
1:A:125:THR:CG2	4:D:76:ARG:HE	2.32	0.42
3:C:95:THR:HG23	3:C:96:GLN:N	2.34	0.42
1:A:277:THR:HG21	4:D:63:GLN:HB2	2.01	0.42
1:A:407:PRO:O	1:A:408:ASP:C	2.63	0.42
3:C:96:GLN:HB3	4:D:9:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:HIS:CD2	1:A:250:HIS:C	2.98	0.42
1:A:125:THR:HG21	4:D:76:ARG:HE	1.83	0.42
1:A:126:MET:HB3	4:D:77:VAL:HB	2.02	0.42
1:A:37:LYS:HE2	3:C:17:VAL:O	2.20	0.42
1:A:15:LYS:HE3	1:A:15:LYS:HB2	1.84	0.41
1:A:61:LEU:HD12	1:A:94:LEU:HD11	2.01	0.41
1:A:301:ASP:HA	1:A:302:PRO:HD3	1.79	0.41
1:A:368:LEU:HD12	1:A:374:ARG:CG	2.51	0.41
1:A:409:ILE:HG23	1:A:470:VAL:HG22	2.02	0.41
1:A:49:CYS:SG	1:A:51:GLU:HB2	2.60	0.41
4:D:11:ILE:HD13	4:D:16:ILE:HG22	2.01	0.41
1:A:140:ILE:HG23	2:B:66:GLU:OE1	2.20	0.41
1:A:41:LEU:HG	3:C:17:VAL:HG11	2.02	0.41
1:A:414:ILE:HD12	4:D:69:LEU:HD11	2.01	0.41
1:A:310:ILE:HD11	1:A:362:LEU:HB3	2.03	0.41
1:A:37:LYS:HE3	1:A:37:LYS:HB2	1.80	0.41
1:A:183:PHE:CE1	1:A:244:PHE:HE2	2.39	0.41
1:A:69:TRP:CD1	1:A:69:TRP:C	2.99	0.41
1:A:96:CYS:HB2	1:A:103:ILE:HD11	2.02	0.41
1:A:105:ASN:OD1	2:B:36:GLN:HG2	2.21	0.41
4:D:42:THR:HG23	4:D:43:PRO:HD2	2.01	0.41
1:A:28:ARG:O	1:A:31:LEU:HB2	2.21	0.40
1:A:322:SER:C	1:A:324:HIS:N	2.80	0.40
4:D:83:LYS:HA	4:D:84:PRO:HD3	1.95	0.40
1:A:183:PHE:O	1:A:186:ALA:HB3	2.21	0.40
2:B:21:THR:O	2:B:25:GLN:HG3	2.21	0.40
4:D:11:ILE:O	4:D:12:LYS:C	2.62	0.40
1:A:174:CYS:O	1:A:176:VAL:N	2.54	0.40
1:A:314:LYS:O	1:A:380:ILE:HA	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	408/471 (87%)	337 (83%)	57 (14%)	14 (3%)	3	7
2	B	87/99 (88%)	75 (86%)	11 (13%)	1 (1%)	11	29
3	C	89/96 (93%)	83 (93%)	4 (4%)	2 (2%)	5	14
4	D	80/104 (77%)	68 (85%)	10 (12%)	2 (2%)	4	11
All	All	664/770 (86%)	563 (85%)	82 (12%)	19 (3%)	3	9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	105	ASN
1	A	130	MET
1	A	212	ARG
1	A	443	ASN
3	C	95	THR
4	D	20	SER
4	D	66	GLU
1	A	68	CYS
1	A	246	ILE
2	B	57	ASP
3	C	8	LEU
1	A	175	LYS
1	A	210	THR
1	A	314	LYS
1	A	119	ASP
1	A	81	ILE
1	A	346	ILE
1	A	423	VAL

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	A	386/429 (90%)	360 (93%)	26 (7%)	15	36
2	B	81/89 (91%)	79 (98%)	2 (2%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	86/91 (94%)	78 (91%)	8 (9%)	8	21
4	D	78/90 (87%)	69 (88%)	9 (12%)	5	14
All	All	631/699 (90%)	586 (93%)	45 (7%)	13	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	7	ILE
1	A	14	GLU
1	A	87	ILE
1	A	91	ASN
1	A	105	ASN
1	A	108	LEU
1	A	127	VAL
1	A	155	LEU
1	A	156	ILE
1	A	173	ASN
1	A	181	LYS
1	A	188	ASP
1	A	192	HIS
1	A	194	LEU
1	A	227	ASN
1	A	246	ILE
1	A	270	GLN
1	A	272	GLU
1	A	274	ILE
1	A	307	SER
1	A	364	ARG
1	A	384	THR
1	A	414	ILE
1	A	438	GLN
1	A	450	ILE
2	B	53	ASN
2	B	79	ASP
3	C	12	ILE
3	C	13	GLN
3	C	24	LEU
3	C	54	GLU
3	C	59	THR
3	C	60	GLN

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Mol	Chain	Res	Type
3	C	70	LEU
3	C	80	THR
4	D	9	LYS
4	D	17	GLU
4	D	21	LEU
4	D	45	GLN
4	D	47	ASP
4	D	49	MET
4	D	51	ARG
4	D	87	LEU
4	D	96	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	13	ASN
1	A	33	HIS
1	A	50	HIS
1	A	53	ASN
1	A	88	ASN
1	A	90	ASN
1	A	91	ASN
1	A	227	ASN
1	A	239	HIS
1	A	251	GLN
1	A	348	GLN
1	A	373	ASN
1	A	438	GLN
2	B	17	ASN
2	B	69	GLN
2	B	75	ASN
3	C	7	GLN
3	C	21	ASN
3	C	35	GLN
3	C	53	ASN
3	C	84	GLN
4	D	48	HIS

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 7 ligands modelled in this entry, 7 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	422/471 (89%)	0.67	36 (8%) 16 14	38, 67, 126, 194	0
2	B	89/99 (89%)	0.70	7 (7%) 18 16	51, 75, 111, 123	0
3	C	91/96 (94%)	0.63	4 (4%) 39 35	54, 76, 123, 129	0
4	D	84/104 (80%)	0.63	2 (2%) 59 56	46, 60, 133, 140	0
All	All	686/770 (89%)	0.66	49 (7%) 22 19	38, 69, 128, 194	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	ALA	5.0
1	A	183	PHE	4.3
1	A	176	VAL	3.8
1	A	198	LEU	3.8
3	C	8	LEU	3.7
1	A	406	VAL	3.6
1	A	54	SER	3.6
2	B	77	GLY	3.5
3	C	6	ALA	3.4
4	D	21	LEU	3.4
1	A	256	ASP	3.4
1	A	271	CYS	3.3
1	A	3	ILE	3.3
1	A	227	ASN	3.1
1	A	235	GLN	3.1
2	B	8	ILE	3.1
1	A	96	CYS	3.1
1	A	261	LYS	3.0
4	D	19	TYR	3.0
1	A	369	LEU	2.9
1	A	226	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	2.8
1	A	175	LYS	2.8
1	A	301	ASP	2.8
1	A	174	CYS	2.7
1	A	375	LYS	2.6
2	B	54	GLY	2.6
1	A	209	SER	2.5
2	B	62	GLN	2.5
1	A	372	SER	2.5
1	A	345	ALA	2.4
1	A	295	ASN	2.4
1	A	272	GLU	2.4
1	A	374	ARG	2.3
1	A	333	ASN	2.3
2	B	66	GLU	2.2
1	A	120	ASP	2.2
1	A	368	LEU	2.2
1	A	225	LYS	2.2
1	A	238	ALA	2.2
2	B	7	THR	2.2
1	A	52	ILE	2.2
1	A	332	PHE	2.1
2	B	92	CYS	2.1
3	C	11	GLN	2.0
1	A	313	LYS	2.0
1	A	328	GLN	2.0
1	A	371	GLY	2.0
3	C	12	ILE	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	A	472	1/1	0.84	0.13	126,126,126,126	0
5	ZN	A	475	1/1	0.86	0.17	107,107,107,107	0
5	ZN	B	100	1/1	0.89	0.12	146,146,146,146	0
5	ZN	A	474	1/1	0.92	0.08	93,93,93,93	0
5	ZN	A	473	1/1	0.93	0.08	89,89,89,89	0
5	ZN	A	476	1/1	0.94	0.07	81,81,81,81	0
5	ZN	D	105	1/1	0.95	0.07	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.