



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:02 PM UTC

PDB ID : 4FIP / pdb_00004fip
Title : Structure of the SAGA Ubp8(S144N)/Sgf11(1-72, Delta-ZnF)/Sus1/Sgf73 DUB module
Authors : Samara, N.L.; Ringel, A.E.; Wolberger, C.
Deposited on : 2012-06-10
Resolution : 2.69 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:

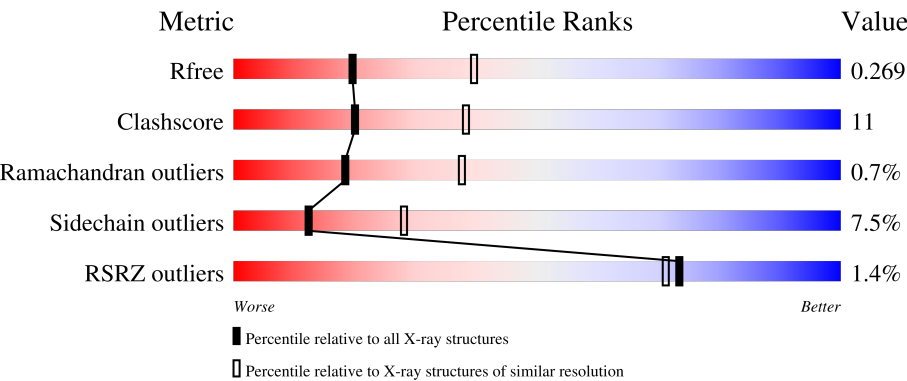
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.69 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	A	476	% 72%18%• 5%
1	E	476	% 66%24%• 7%
2	B	96	% 69%22%• 6%
2	F	96	2% 71%19%• 6%
3	C	72	40%11%6%43%

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Mol	Chain	Length	Quality of chain
3	G	72	
4	D	96	
4	H	96	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10730 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	450	Total	C	N	O	S	0	0	0
			3597	2276	618	667	36			
1	E	441	Total	C	N	O	S	0	0	0
			3534	2244	603	651	36			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P50102
A	-3	ALA	-	expression tag	UNP P50102
A	-2	ALA	-	expression tag	UNP P50102
A	-1	ALA	-	expression tag	UNP P50102
A	0	ALA	-	expression tag	UNP P50102
A	144	ASN	SER	engineered mutation	UNP P50102
E	-4	GLY	-	expression tag	UNP P50102
E	-3	ALA	-	expression tag	UNP P50102
E	-2	ALA	-	expression tag	UNP P50102
E	-1	ALA	-	expression tag	UNP P50102
E	0	ALA	-	expression tag	UNP P50102
E	144	ASN	SER	engineered mutation	UNP P50102

- Molecule 2 is a protein called Protein SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			727	455	119	151	2			
2	F	90	Total	C	N	O	S	0	1	0
			735	460	122	151	2			

- Molecule 3 is a protein called SAGA-associated factor 11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	41	Total	C	N	O	0	0	0
			324	203	55	66			
3	G	43	Total	C	N	O	0	0	0
			342	213	57	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	88	Total	C	N	O	S	0	0	0
			695	439	115	137	4			
4	H	83	Total	C	N	O	S	1	0	0
			670	426	111	129	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Zn	0	0
			6	6		
5	D	1	Total	Zn	0	0
			1	1		
5	E	6	Total	Zn	0	0
			6	6		
5	H	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total	O	0	0
			34	34		
6	B	3	Total	O	0	0
			3	3		
6	C	1	Total	O	0	0
			1	1		
6	D	11	Total	O	0	0
			11	11		
6	E	34	Total	O	0	0
			34	34		
6	F	5	Total	O	0	0
			5	5		
6	G	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	3	Total	O	0	0
			3	3		

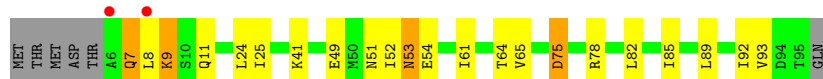
- Molecule 2: Protein SUS1

Chain B:  69% 22% 6%



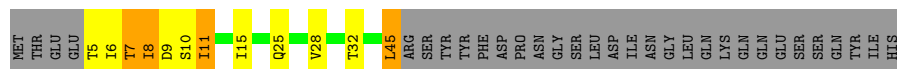
- Molecule 2: Protein SUS1

Chain F:  71% 19% 6%



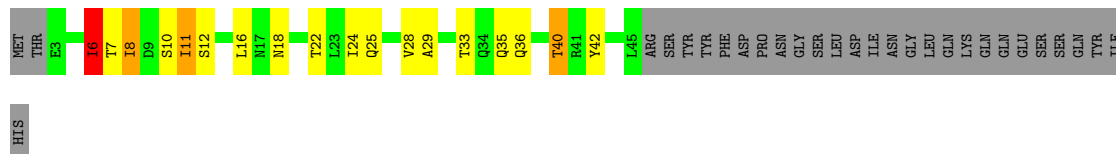
- Molecule 3: SAGA-associated factor 11

Chain C:  40% 11% 6% 43%



- Molecule 3: SAGA-associated factor 11

Chain G:  35% 19% 40% 2%



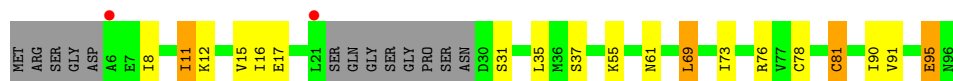
- Molecule 4: SAGA-associated factor 73

Chain D:  74% 16% 8% 2%



- Molecule 4: SAGA-associated factor 73

Chain H:  67% 16% 14% 2%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 79.97Å 274.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.69 47.18 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.0 (47.18-2.69) 91.0 (47.18-2.69)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.264 0.188 , 0.269	Depositor DCC
R_{free} test set	2199 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10730	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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	1.02	5/3674 (0.1%)	1.00	6/4950 (0.1%)
1	E	0.96	0/3612	1.00	3/4867 (0.1%)
2	B	0.82	0/733	1.02	0/988
2	F	0.82	0/744	1.02	1/1002 (0.1%)
3	C	0.95	0/325	1.10	0/443
3	G	0.77	0/343	0.98	0/467
4	D	1.03	1/708 (0.1%)	1.07	0/954
4	H	0.98	1/683 (0.1%)	1.04	1/919 (0.1%)
All	All	0.96	7/10822 (0.1%)	1.01	11/14590 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	HIS	CG-CD2	5.83	1.42	1.35
4	D	93	HIS	CG-CD2	5.54	1.42	1.35
1	A	198	LEU	CA-C	5.21	1.57	1.53
1	A	324	HIS	CG-CD2	5.19	1.41	1.35
4	H	95	GLU	C-O	5.15	1.30	1.24
1	A	237	ASP	N-CA	5.05	1.52	1.46
1	A	250	HIS	CG-ND1	-5.02	1.32	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	N-CA-C	6.17	118.33	108.41
1	A	140	ILE	CB-CA-C	-6.09	104.66	111.23
1	A	178	SER	CA-C-N	5.89	125.59	119.05
1	A	178	SER	C-N-CA	5.89	125.59	119.05
1	E	80	GLN	CA-C-N	5.74	132.03	121.70
1	E	80	GLN	C-N-CA	5.74	132.03	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	81	CYS	CB-CA-C	-5.53	102.19	110.88
2	F	65	VAL	N-CA-C	5.36	116.77	111.67
1	E	81	ILE	N-CA-C	5.35	125.98	111.00
1	A	245	ILE	CB-CA-C	-5.28	105.21	111.97
1	A	215	GLY	N-CA-C	-5.09	106.60	112.50

There are no chirality outliers.

There are no planarity outliers.

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	3597	0	3504	72	0
1	E	3534	0	3445	99	0
2	B	727	0	734	18	0
2	F	735	0	747	20	0
3	C	324	0	341	15	0
3	G	342	0	353	28	0
4	D	695	0	685	14	0
4	H	670	0	672	13	0
5	A	6	0	0	0	0
5	D	1	0	0	0	0
5	E	6	0	0	0	0
5	H	1	0	0	0	0
6	A	34	0	0	0	0
6	B	3	0	0	0	0
6	C	1	0	0	0	0
6	D	11	0	0	0	0
6	E	34	0	0	1	0
6	F	5	0	0	0	0
6	G	1	0	0	0	0
6	H	3	0	0	0	0
All	All	10730	0	10481	240	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 (240) 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:F:89:LEU:HD11	3:G:11:ILE:HD11	1.20	1.19
1:E:105:ASN:HD22	3:G:40:THR:HG21	1.03	1.09
3:G:36:GLN:O	3:G:40:THR:HG23	1.60	1.02
1:E:142:MET:HE1	1:E:231:ALA:HB1	1.38	1.01
2:B:12:ILE:HG22	4:D:11:ILE:HD11	1.47	0.96
1:A:251:GLN:O	1:A:255:LEU:HD13	1.65	0.95
4:H:12:LYS:O	4:H:15:VAL:HG22	1.66	0.94
1:E:142:MET:CE	1:E:231:ALA:HB1	2.01	0.91
2:F:93:VAL:HG11	3:G:8:ILE:HD11	1.55	0.89
2:F:61:ILE:O	2:F:64:THR:HG22	1.73	0.89
2:F:93:VAL:HG11	3:G:8:ILE:CD1	2.04	0.87
1:E:105:ASN:ND2	3:G:40:THR:HG21	1.89	0.87
1:E:148:MET:HE3	1:E:241:PHE:CE1	2.10	0.85
1:E:287:ILE:CG2	1:E:345:ALA:HB1	2.07	0.85
2:B:12:ILE:HD13	2:B:89:LEU:HD21	1.62	0.81
2:F:89:LEU:CD1	3:G:11:ILE:HD11	2.08	0.81
1:A:213:GLN:HE22	1:E:139:LEU:HA	1.45	0.80
2:B:12:ILE:HD13	2:B:89:LEU:CD2	2.13	0.79
2:B:41:LYS:HB3	2:B:72:MET:HE1	1.64	0.77
2:B:41:LYS:HB3	2:B:72:MET:CE	2.18	0.73
3:G:11:ILE:HD12	3:G:11:ILE:C	2.12	0.73
3:C:7:THR:HG23	3:C:10:SER:HB3	1.71	0.72
1:A:148:MET:HE1	1:A:220:LEU:HD21	1.73	0.70
3:G:11:ILE:HD12	3:G:12:SER:N	2.06	0.70
1:E:320:LEU:O	1:E:323:PHE:HB3	1.91	0.70
1:A:148:MET:HE1	1:A:220:LEU:CD2	2.21	0.69
2:B:8:LEU:O	2:B:12:ILE:HG23	1.93	0.69
1:A:376:LEU:HD12	1:A:376:LEU:N	2.07	0.69
1:E:142:MET:HE1	1:E:231:ALA:CB	2.21	0.68
1:E:235:GLN:OE1	1:E:423:VAL:HG12	1.93	0.67
2:F:89:LEU:HD11	3:G:11:ILE:CD1	2.13	0.67
2:B:32:ARG:NH1	2:B:80:THR:HG21	2.10	0.67
1:A:171:SER:O	1:A:177:ARG:NH1	2.28	0.66
1:E:379:PHE:C	1:E:380:ILE:HD12	2.20	0.66
1:E:287:ILE:HG22	1:E:345:ALA:HB1	1.77	0.66
1:E:140:ILE:CD1	1:E:142:MET:CE	2.74	0.65
1:E:71:HIS:HB2	1:E:73:HIS:CE1	2.31	0.65
1:E:140:ILE:CD1	1:E:142:MET:HE3	2.27	0.64
1:E:224:TRP:CD1	1:E:231:ALA:HB2	2.32	0.64
1:E:416:ILE:HD12	1:E:455:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:SER:O	1:A:325:LYS:HD2	1.98	0.64
1:E:156:ILE:O	1:E:162:ILE:HD11	1.98	0.63
1:A:20:VAL:HG13	1:A:61:LEU:HD21	1.81	0.62
2:B:12:ILE:HD11	3:C:15:ILE:HD11	1.82	0.61
2:B:12:ILE:CD1	2:B:89:LEU:HD21	2.29	0.61
3:C:11:ILE:HD12	3:C:11:ILE:O	2.01	0.61
1:E:140:ILE:HD11	1:E:142:MET:HE1	1.82	0.61
1:A:156:ILE:C	1:A:156:ILE:HD12	2.26	0.61
4:H:11:ILE:HG23	4:H:15:VAL:CG2	2.30	0.61
1:A:141:ASN:HD22	1:E:145:THR:HB	1.67	0.60
1:E:287:ILE:HG23	1:E:345:ALA:HB1	1.82	0.60
2:F:89:LEU:O	2:F:93:VAL:HG12	2.01	0.60
2:F:25:ILE:HD13	2:F:85:ILE:HG12	1.84	0.60
1:A:1:MET:HE2	1:A:2:SER:H	1.66	0.60
4:D:12:LYS:O	4:D:15:VAL:HG12	2.01	0.59
1:A:246:ILE:HD12	1:A:304:LEU:HD13	1.84	0.59
1:A:286:SER:HA	1:A:298:THR:HG22	1.84	0.59
1:A:142:MET:CE	1:A:224:TRP:HB2	2.33	0.58
1:E:52:ILE:HD13	1:E:52:ILE:N	2.17	0.58
1:E:268:ASN:N	1:E:269:LYS:HA	2.18	0.58
1:A:292:CYS:O	1:A:293:GLN:HB2	2.04	0.58
1:A:288:VAL:HG12	1:A:289:CYS:O	2.04	0.57
4:D:38:SER:O	4:D:42:THR:OG1	2.22	0.57
1:E:148:MET:HE3	1:E:241:PHE:HE1	1.68	0.57
3:G:7:THR:HG22	3:G:10:SER:HB2	1.86	0.57
1:A:274:ILE:O	1:A:278:VAL:HG13	2.04	0.57
1:A:148:MET:CE	1:A:220:LEU:HD21	2.34	0.57
4:H:15:VAL:C	4:H:17:GLU:H	2.13	0.57
1:E:152:LEU:HD11	1:E:219:LEU:CD2	2.34	0.57
4:D:48:HIS:NE2	4:D:67:ASP:OD1	2.37	0.56
1:E:375:LYS:NZ	1:E:421:GLY:O	2.35	0.56
2:F:75:ASP:N	2:F:75:ASP:OD1	2.39	0.56
3:C:6:ILE:HG22	3:C:6:ILE:O	2.05	0.56
2:B:57:ASN:HD22	2:B:60:GLN:H	1.55	0.55
1:E:140:ILE:HD11	1:E:142:MET:CE	2.37	0.55
2:F:93:VAL:CG1	3:G:8:ILE:HD11	2.33	0.55
1:A:156:ILE:HD12	1:A:157:HIS:ND1	2.21	0.55
1:E:335:HIS:HE1	1:E:340:ASN:HD22	1.53	0.55
3:G:7:THR:CG2	3:G:10:SER:HB2	2.37	0.55
1:E:162:ILE:CG2	1:E:166:MET:HE3	2.37	0.55
2:F:7:GLN:CD	2:F:7:GLN:O	2.50	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:CYS:HB2	1:E:68:CYS:HB3	1.89	0.54
1:E:148:MET:CE	1:E:241:PHE:CE1	2.86	0.54
1:A:56:ALA:H	3:C:25:GLN:NE2	2.05	0.54
1:A:142:MET:HE1	1:A:224:TRP:CB	2.36	0.54
1:E:284:GLU:HB2	1:E:352:HIS:HB2	1.90	0.54
2:F:7:GLN:O	2:F:7:GLN:CG	2.54	0.54
3:C:28:VAL:O	3:C:32:THR:HG23	2.06	0.54
1:A:376:LEU:N	1:A:376:LEU:CD1	2.71	0.54
2:F:78[A]:ARG:HG2	2:F:82:LEU:HD12	1.89	0.54
1:A:42:ASN:HB2	4:D:35:LEU:HD11	1.89	0.54
2:B:89:LEU:HD11	3:C:11:ILE:HD11	1.89	0.53
3:G:24:ILE:O	3:G:28:VAL:HG23	2.08	0.53
1:A:334:TYR:O	1:A:342:THR:HG22	2.09	0.53
1:E:287:ILE:CG2	1:E:345:ALA:CB	2.84	0.53
1:E:140:ILE:CD1	1:E:142:MET:HE1	2.38	0.53
3:G:36:GLN:O	3:G:40:THR:CG2	2.46	0.53
3:C:9:ASP:OD2	4:D:5:ASP:N	2.42	0.53
1:A:224:TRP:CE2	1:E:217:ILE:HG21	2.43	0.52
1:A:366:GLU:OE2	1:A:374:ARG:NH2	2.43	0.52
4:H:12:LYS:HB2	4:H:15:VAL:HG13	1.91	0.52
4:D:49:MET:HE3	6:E:601:HOH:O	2.10	0.52
2:F:82:LEU:HG	3:G:16:LEU:HD22	1.92	0.52
1:A:142:MET:HE3	1:A:224:TRP:HB2	1.91	0.51
3:C:7:THR:CG2	3:C:10:SER:HB3	2.37	0.51
1:E:42:ASN:HB3	4:H:35:LEU:HD11	1.92	0.51
1:E:48:THR:HG21	1:E:73:HIS:CD2	2.46	0.51
1:A:88:ASN:HB3	1:A:91:ASN:OD1	2.10	0.51
1:E:141:ASN:HD22	1:E:143:GLY:H	1.58	0.51
1:A:324:HIS:CG	1:A:324:HIS:O	2.62	0.51
1:A:452:GLN:O	1:A:453:GLU:C	2.54	0.50
4:D:21:LEU:C	4:D:21:LEU:CD2	2.85	0.50
1:A:384:THR:CG2	1:A:456:LEU:HD11	2.41	0.50
3:G:6:ILE:O	3:G:6:ILE:HG13	2.12	0.50
1:E:42:ASN:CB	4:H:35:LEU:HD11	2.41	0.50
1:A:77:HIS:O	1:A:81:ILE:HG22	2.11	0.50
4:D:46:TYR:HB2	4:D:49:MET:HB2	1.93	0.49
1:E:4:CYS:HB3	1:E:7:ILE:HG22	1.94	0.49
1:A:366:GLU:HG3	1:A:376:LEU:HD11	1.93	0.49
1:A:246:ILE:CD1	1:A:304:LEU:HD13	2.43	0.49
1:E:71:HIS:CB	1:E:73:HIS:CE1	2.96	0.49
1:E:351:ILE:HD12	1:E:391:TYR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ILE:HD12	1:E:380:ILE:N	2.28	0.49
1:A:21:LEU:HD13	1:A:108:LEU:HD11	1.94	0.49
1:E:16:SER:O	1:E:20:VAL:HG13	2.13	0.49
1:A:247:ASN:O	1:A:251:GLN:HG2	2.13	0.48
1:E:140:ILE:HD12	1:E:142:MET:CE	2.43	0.48
1:E:416:ILE:HD12	1:E:455:VAL:CG1	2.43	0.48
3:G:7:THR:HG23	3:G:10:SER:N	2.28	0.48
1:E:140:ILE:HG13	1:E:142:MET:HE3	1.96	0.48
1:E:334:TYR:CE1	1:E:345:ALA:HB2	2.49	0.48
1:A:148:MET:HE1	1:A:220:LEU:HD23	1.93	0.48
3:C:6:ILE:HG23	3:C:11:ILE:CG2	2.43	0.48
3:C:45:LEU:N	3:C:45:LEU:HD12	2.28	0.48
1:E:141:ASN:O	1:E:232:GLY:HA2	2.14	0.48
1:A:142:MET:HE1	1:A:224:TRP:HB3	1.95	0.48
1:A:287:ILE:N	1:A:287:ILE:HD12	2.28	0.48
1:E:242:TRP:O	1:E:245:ILE:HG22	2.13	0.48
1:E:23:THR:CG2	1:E:61:LEU:HD12	2.44	0.48
1:A:141:ASN:HB3	1:E:145:THR:HG21	1.97	0.47
1:E:180:ASP:OD1	1:E:180:ASP:N	2.45	0.47
1:E:141:ASN:ND2	1:E:143:GLY:H	2.13	0.46
1:E:373:ASN:HB2	1:E:423:VAL:HG11	1.97	0.46
1:A:220:LEU:HD13	1:E:142:MET:HG3	1.97	0.46
1:A:263:VAL:O	1:A:267:ASN:HB2	2.15	0.46
1:A:261:LYS:HG3	1:A:262:GLU:N	2.31	0.46
1:E:128:PRO:O	3:G:42:TYR:OH	2.31	0.46
3:C:6:ILE:O	4:D:8:ILE:HD13	2.16	0.46
1:A:170:HIS:CE1	1:A:184:SER:HB2	2.49	0.46
1:E:3:ILE:HG22	1:E:4:CYS:N	2.31	0.46
1:E:74:PHE:CD1	1:E:97:PHE:CE2	3.04	0.46
4:H:91:VAL:HG12	4:H:95:GLU:HG3	1.98	0.46
3:C:11:ILE:HD12	3:C:11:ILE:C	2.41	0.46
1:E:354:LEU:HB3	1:E:411:TYR:OH	2.16	0.46
1:E:152:LEU:HD11	1:E:219:LEU:HD22	1.97	0.45
1:E:158:ASN:HD21	1:E:357:VAL:HG21	1.80	0.45
1:E:251:GLN:O	1:E:255:LEU:HD13	2.16	0.45
1:A:50:HIS:O	2:B:10:SER:HB2	2.17	0.45
1:A:416:ILE:HD12	1:A:455:VAL:HG13	1.99	0.45
1:E:80:GLN:HA	1:E:82:GLY:N	2.31	0.45
2:F:25:ILE:CD1	2:F:85:ILE:HG12	2.47	0.45
2:F:8:LEU:O	2:F:11:GLN:N	2.42	0.45
1:A:221:THR:HG21	1:E:225:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:GLU:N	2:B:67:PRO:CD	2.81	0.44
1:A:4:CYS:HB3	1:A:7:ILE:HG22	1.99	0.44
1:A:323:PHE:CD1	1:A:323:PHE:C	2.94	0.44
1:E:35:VAL:HG13	1:E:36:PRO:HD2	1.99	0.44
1:A:216:PHE:HE2	1:E:140:ILE:O	2.00	0.44
1:E:93:LEU:HD13	3:G:33:THR:HG21	2.00	0.44
1:A:286:SER:HA	1:A:298:THR:CG2	2.48	0.44
1:E:253:TYR:CG	1:E:273:CYS:HB3	2.53	0.44
3:G:29:ALA:O	3:G:33:THR:HG23	2.18	0.44
1:A:142:MET:HE1	1:A:224:TRP:HB2	1.99	0.43
1:E:274:ILE:CD1	1:E:278:VAL:HG21	2.48	0.43
4:D:73:ILE:HD12	4:D:73:ILE:H	1.82	0.43
1:E:368:LEU:HD12	1:E:372:SER:O	2.18	0.43
4:D:21:LEU:C	4:D:21:LEU:HD23	2.43	0.43
1:E:56:ALA:H	3:G:25:GLN:NE2	2.16	0.43
1:E:213:GLN:N	1:E:213:GLN:OE1	2.52	0.43
1:E:23:THR:HG22	1:E:61:LEU:HD12	1.98	0.43
1:A:446:MET:HE2	1:A:448:SER:HB3	2.00	0.43
3:C:7:THR:HG23	3:C:10:SER:H	1.84	0.43
1:A:287:ILE:HD13	1:A:297:LYS:O	2.19	0.43
1:A:375:LYS:NZ	1:A:459:GLN:HE22	2.16	0.43
3:G:6:ILE:O	4:H:8:ILE:HB	2.18	0.43
1:A:296:SER:HA	1:A:297:LYS:HA	1.62	0.43
1:E:444:ASP:HA	1:E:445:SER:HA	1.81	0.43
3:G:8:ILE:HA	4:H:8:ILE:HD11	2.01	0.43
1:A:140:ILE:HD12	1:E:213:GLN:H	1.83	0.43
4:D:48:HIS:HE2	4:D:67:ASP:CG	2.26	0.43
1:A:295:ASN:O	1:A:298:THR:HG23	2.19	0.42
1:E:162:ILE:HG23	1:E:166:MET:HE3	2.00	0.42
3:C:8:ILE:N	4:D:8:ILE:HD11	2.34	0.42
1:E:71:HIS:HB2	1:E:73:HIS:ND1	2.34	0.42
1:A:156:ILE:CD1	1:A:157:HIS:CE1	3.02	0.42
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.70	0.42
2:B:75:ASP:O	2:B:79:GLU:HG2	2.19	0.42
1:E:90:ASN:HD21	3:G:22:THR:HG23	1.84	0.42
1:E:140:ILE:HD12	1:E:142:MET:HE3	1.99	0.42
1:A:158:ASN:HA	1:A:159:PRO:HD3	1.82	0.42
1:E:413:LEU:HB2	1:E:465:TYR:CE1	2.55	0.42
2:F:7:GLN:O	2:F:7:GLN:HG3	2.18	0.42
2:F:78[B]:ARG:HG2	3:G:16:LEU:HD21	2.01	0.42
2:B:41:LYS:HB3	2:B:72:MET:HE3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:CYS:HB3	1:E:341:SER:OG	2.19	0.42
1:A:433:LYS:HD2	4:H:69:LEU:HD12	2.02	0.42
1:A:176:VAL:HG12	1:A:178:SER:H	1.85	0.41
1:E:316:LEU:HD21	1:E:360:LEU:CD1	2.50	0.41
4:H:78:CYS:HB3	4:H:81:CYS:HB2	2.01	0.41
1:E:222:CYS:O	1:E:226:ILE:HG13	2.20	0.41
1:E:25:ASN:O	1:E:26:ALA:C	2.63	0.41
2:B:46:THR:HG22	2:B:50:MET:HE2	2.02	0.41
1:A:221:THR:HG21	1:E:225:LYS:NZ	2.35	0.41
1:A:382:PHE:CE2	1:A:456:LEU:HD23	2.55	0.41
1:E:140:ILE:CG1	1:E:142:MET:HE3	2.50	0.41
1:E:301:ASP:HA	1:E:302:PRO:HD2	1.87	0.41
1:E:3:ILE:CG2	1:E:106:ILE:HD11	2.51	0.41
1:E:108:LEU:HD13	1:E:118:TRP:CG	2.56	0.41
1:A:103:ILE:CG2	1:A:106:ILE:HD12	2.51	0.41
1:A:283:LEU:HA	1:A:283:LEU:HD23	1.81	0.41
2:B:73:VAL:HG22	2:B:78:ARG:NH1	2.36	0.41
1:E:53:ASN:O	3:G:18:ASN:HB3	2.20	0.41
1:E:54:SER:HB3	1:E:68:CYS:HB2	2.03	0.41
1:E:183:PHE:O	1:E:186:ALA:HB3	2.21	0.41
1:E:382:PHE:HA	1:E:383:PRO:HD3	1.98	0.41
1:E:411:TYR:HB3	1:E:465:TYR:HB3	2.03	0.41
4:H:11:ILE:HG23	4:H:15:VAL:HG22	2.02	0.41
1:A:460:ALA:CB	1:A:463:LEU:HD21	2.51	0.41
1:E:374:ARG:HD2	1:E:375:LYS:N	2.36	0.41
2:F:53:ASN:O	2:F:54:GLU:C	2.64	0.41
1:A:211:ASN:HB3	1:A:213:GLN:HB2	2.02	0.40
1:A:216:PHE:HB2	1:E:139:LEU:HD22	2.04	0.40
1:E:158:ASN:HA	1:E:159:PRO:HD3	1.85	0.40
3:G:11:ILE:C	3:G:11:ILE:CD1	2.85	0.40
2:B:22:TYR:O	2:B:23:GLU:C	2.63	0.40
1:E:81:ILE:O	1:E:81:ILE:HG23	2.19	0.40
1:A:21:LEU:HD11	1:A:108:LEU:HG	2.04	0.40
1:A:467:ILE:O	1:A:467:ILE:HG23	2.22	0.40
2:F:49:GLU:HG3	2:F:64:THR:HG23	2.03	0.40
4:H:76:ARG:HB2	4:H:90:ILE:HD11	2.03	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	442/476 (93%)	418 (95%)	22 (5%)	2 (0%)	24	45
1	E	433/476 (91%)	408 (94%)	22 (5%)	3 (1%)	18	37
2	B	88/96 (92%)	86 (98%)	2 (2%)	0	100	100
2	F	89/96 (93%)	81 (91%)	7 (8%)	1 (1%)	11	26
3	C	39/72 (54%)	38 (97%)	1 (3%)	0	100	100
3	G	41/72 (57%)	39 (95%)	1 (2%)	1 (2%)	4	10
4	D	82/96 (85%)	78 (95%)	3 (4%)	1 (1%)	10	24
4	H	79/96 (82%)	75 (95%)	3 (4%)	1 (1%)	9	22
All	All	1293/1480 (87%)	1223 (95%)	61 (5%)	9 (1%)	18	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	371	GLY
4	H	16	ILE
1	A	293	GLN
1	A	332	PHE
4	D	31	SER
1	E	72	SER
1	E	339	CYS
2	F	9	LYS
3	G	6	ILE

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	410/429 (96%)	381 (93%)	29 (7%)	13	30
1	E	403/429 (94%)	377 (94%)	26 (6%)	15	34
2	B	85/91 (93%)	78 (92%)	7 (8%)	10	24
2	F	86/91 (94%)	77 (90%)	9 (10%)	6	15
3	C	39/68 (57%)	34 (87%)	5 (13%)	4	9
3	G	41/68 (60%)	36 (88%)	5 (12%)	5	10
4	D	79/86 (92%)	76 (96%)	3 (4%)	29	55
4	H	76/86 (88%)	69 (91%)	7 (9%)	8	19
All	All	1219/1348 (90%)	1128 (92%)	91 (8%)	12	28

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	LYS
1	A	109	ILE
1	A	124	LYS
1	A	142	MET
1	A	178	SER
1	A	220	LEU
1	A	240	GLU
1	A	252	SER
1	A	259	ASN
1	A	261	LYS
1	A	267	ASN
1	A	269	LYS
1	A	278	VAL
1	A	293	GLN
1	A	297	LYS
1	A	305	ASP
1	A	310	ILE
1	A	314	LYS
1	A	323	PHE
1	A	325	LYS
1	A	369	LEU
1	A	376	LEU
1	A	378	ASP
1	A	393	SER

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Mol	Chain	Res	Type
1	A	441	LYS
1	A	446	MET
1	A	453	GLU
1	A	470	VAL
2	B	7	GLN
2	B	8	LEU
2	B	12	ILE
2	B	28	GLU
2	B	51	ASN
2	B	73	VAL
2	B	76	SER
3	C	5	THR
3	C	7	THR
3	C	8	ILE
3	C	11	ILE
3	C	45	LEU
4	D	5	ASP
4	D	21	LEU
4	D	80	LYS
1	E	15	LYS
1	E	20	VAL
1	E	52	ILE
1	E	81	ILE
1	E	124	LYS
1	E	131	GLU
1	E	132	ARG
1	E	142	MET
1	E	145	THR
1	E	156	ILE
1	E	180	ASP
1	E	198	LEU
1	E	243	GLN
1	E	268	ASN
1	E	288	VAL
1	E	299	THR
1	E	320	LEU
1	E	324	HIS
1	E	330	LYS
1	E	369	LEU
1	E	370	ASN
1	E	394	THR
1	E	418	SER

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Mol	Chain	Res	Type
1	E	433	LYS
1	E	453	GLU
1	E	459	GLN
2	F	7	GLN
2	F	9	LYS
2	F	24	LEU
2	F	41	LYS
2	F	51	ASN
2	F	52	ILE
2	F	53	ASN
2	F	75	ASP
2	F	92	ILE
3	G	6	ILE
3	G	8	ILE
3	G	11	ILE
3	G	35	GLN
3	G	40	THR
4	H	11	ILE
4	H	31	SER
4	H	37	SER
4	H	55	LYS
4	H	61	ASN
4	H	69	LEU
4	H	73	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	32	ASN
1	A	42	ASN
1	A	70	ASN
1	A	77	HIS
1	A	90	ASN
1	A	110	ASN
1	A	144	ASN
1	A	153	GLN
1	A	168	GLN
1	A	192	HIS
1	A	213	GLN
1	A	229	ASN
1	A	236	GLN

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Mol	Chain	Res	Type
1	A	250	HIS
1	A	267	ASN
1	A	268	ASN
1	A	276	HIS
1	A	348	GLN
1	A	459	GLN
1	A	469	GLN
2	B	7	GLN
2	B	57	ASN
2	B	84	GLN
3	C	18	ASN
3	C	25	GLN
4	D	29	ASN
1	E	32	ASN
1	E	33	HIS
1	E	50	HIS
1	E	62	GLN
1	E	70	ASN
1	E	90	ASN
1	E	105	ASN
1	E	110	ASN
1	E	141	ASN
1	E	170	HIS
1	E	192	HIS
1	E	227	ASN
1	E	229	ASN
1	E	276	HIS
1	E	293	GLN
1	E	294	ASN
1	E	335	HIS
1	E	340	ASN
2	F	11	GLN
2	F	13	GLN
2	F	27	ASN
2	F	84	GLN
3	G	13	ASN
3	G	25	GLN
3	G	34	GLN
4	H	96	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 14 ligands modelled in this entry, 14 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	450/476 (94%)	-0.34	6 (1%) 75 73	25, 42, 90, 126	0
1	E	441/476 (92%)	-0.25	6 (1%) 73 71	29, 49, 79, 113	0
2	B	90/96 (93%)	-0.34	1 (1%) 78 76	30, 50, 91, 104	0
2	F	90/96 (93%)	-0.11	2 (2%) 62 59	32, 59, 104, 116	1 (1%)
3	C	41/72 (56%)	-0.32	0 100 100	27, 38, 77, 91	0
3	G	43/72 (59%)	-0.20	0 100 100	40, 51, 89, 100	0
4	D	88/96 (91%)	-0.10	2 (2%) 61 57	27, 48, 98, 101	0
4	H	83/96 (86%)	-0.12	2 (2%) 59 56	31, 48, 105, 118	1 (1%)
All	All	1326/1480 (89%)	-0.26	19 (1%) 73 71	25, 47, 92, 126	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	PHE	5.3
4	H	21	LEU	4.2
4	H	6	ALA	3.0
4	D	21	LEU	2.9
1	A	394	THR	2.9
1	E	369	LEU	2.6
1	A	198	LEU	2.5
1	E	368	LEU	2.5
4	D	24	GLY	2.4
2	F	8	LEU	2.4
2	B	6	ALA	2.3
1	E	269	LYS	2.3
1	E	405	LYS	2.3
1	A	140	ILE	2.2
1	A	333	ASN	2.2
2	F	6	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	374	ARG	2.1
1	E	212	ARG	2.0
1	A	331	ASP	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	D	101	1/1	0.98	0.04	47,47,47,47	0
5	ZN	A	506	1/1	0.99	0.04	80,80,80,80	0
5	ZN	A	504	1/1	0.99	0.02	42,42,42,42	0
5	ZN	E	502	1/1	0.99	0.02	39,39,39,39	0
5	ZN	E	503	1/1	0.99	0.02	61,61,61,61	0
5	ZN	E	505	1/1	0.99	0.03	59,59,59,59	0
5	ZN	H	101	1/1	0.99	0.01	45,45,45,45	0
5	ZN	E	501	1/1	1.00	0.01	55,55,55,55	0
5	ZN	A	501	1/1	1.00	0.01	39,39,39,39	0
5	ZN	A	505	1/1	1.00	0.02	56,56,56,56	0
5	ZN	E	504	1/1	1.00	0.02	43,43,43,43	0
5	ZN	A	502	1/1	1.00	0.01	41,41,41,41	0
5	ZN	E	506	1/1	1.00	0.03	59,59,59,59	0
5	ZN	A	503	1/1	1.00	0.01	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.