Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 03:28 AM EDT

PDB ID	:	4W4U
Title	:	Structure of yeast SAGA DUBm with Sgf73 Y57A mutant at 2.8 angstroms resolution
Authors	:	Wolberger, C.; Yan, M.
Deposited on	:	2014-08-15
Resolution	:	2.80 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:

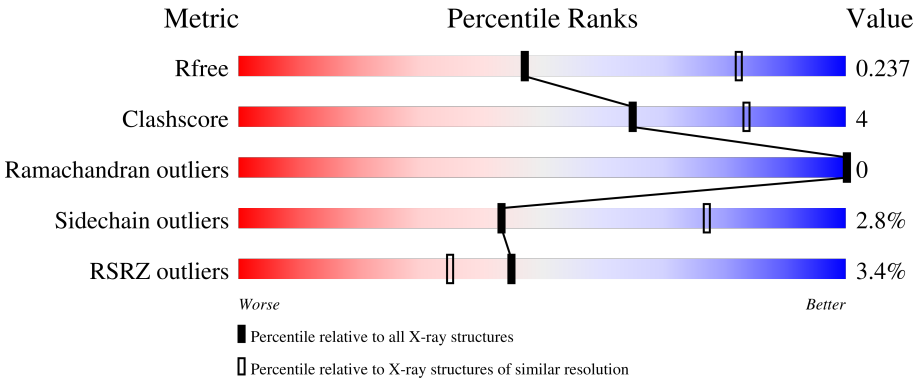
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



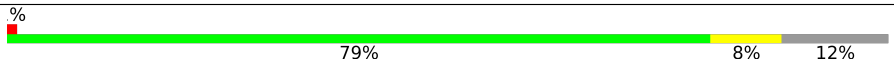
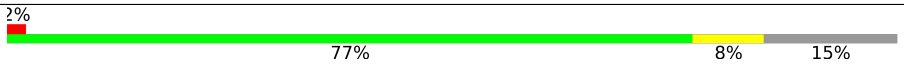
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	4% 80% 11% 8%
1	D	476	4% 76% 10% 14%
2	B	96	% 93% 7%
2	F	96	2% 84% 14%
3	C	99	% 51% 8% 40%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	99	
4	E	96	
4	H	96	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10594 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	4	0
			3526	2245	598	647	36			
1	D	409	Total	C	N	O	S	0	2	0
			3294	2107	557	599	31			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP N1P0J5
A	-3	ALA	-	expression tag	UNP N1P0J5
A	-2	ALA	-	expression tag	UNP N1P0J5
A	-1	ALA	-	expression tag	UNP N1P0J5
A	0	ALA	-	expression tag	UNP N1P0J5
D	-4	GLY	-	expression tag	UNP N1P0J5
D	-3	ALA	-	expression tag	UNP N1P0J5
D	-2	ALA	-	expression tag	UNP N1P0J5
D	-1	ALA	-	expression tag	UNP N1P0J5
D	0	ALA	-	expression tag	UNP N1P0J5

- Molecule 2 is a protein called Transcription and mRNA export factor SUS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	1	0
			780	487	126	163	4			
2	F	94	Total	C	N	O	S	0	1	0
			765	478	124	160	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	59	Total	C	N	O	0	0	0
			471	296	80	95			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	47	Total	C	N	O	S	0	0	0
			374	231	64	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	84	Total	C	N	O	S	0	0	0
			669	422	114	129	4			
4	H	82	Total	C	N	O	S	0	0	0
			649	408	110	127	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	57	ALA	TYR	engineered mutation	UNP P53165
H	57	ALA	TYR	engineered mutation	UNP P53165

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	5	Total	O	0	0
			5	5		
6	E	3	Total	O	0	0
			3	3		
6	D	25	Total	O	0	0
			25	25		
6	F	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

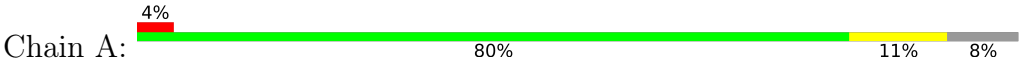
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	2	Total O 2 2	0	0
6	H	6	Total O 6 6	0	0

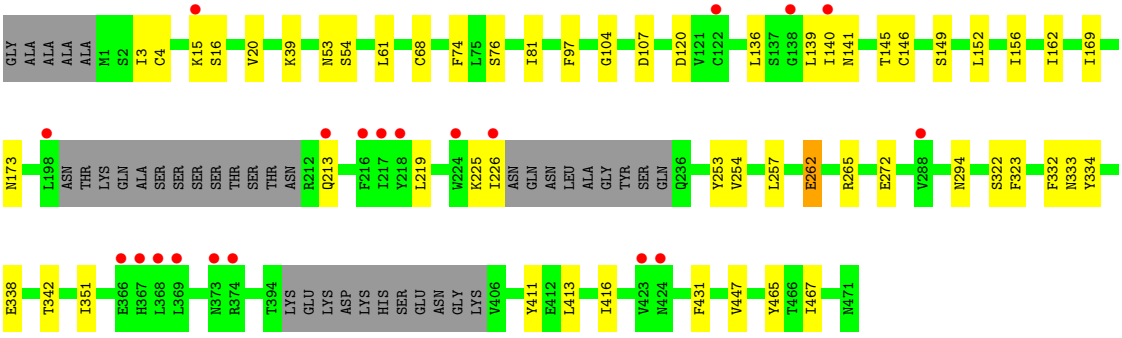
3 Residue-property plots (i)

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: Ubiquitin carboxyl-terminal hydrolase

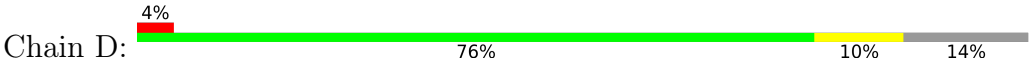
Chain A:

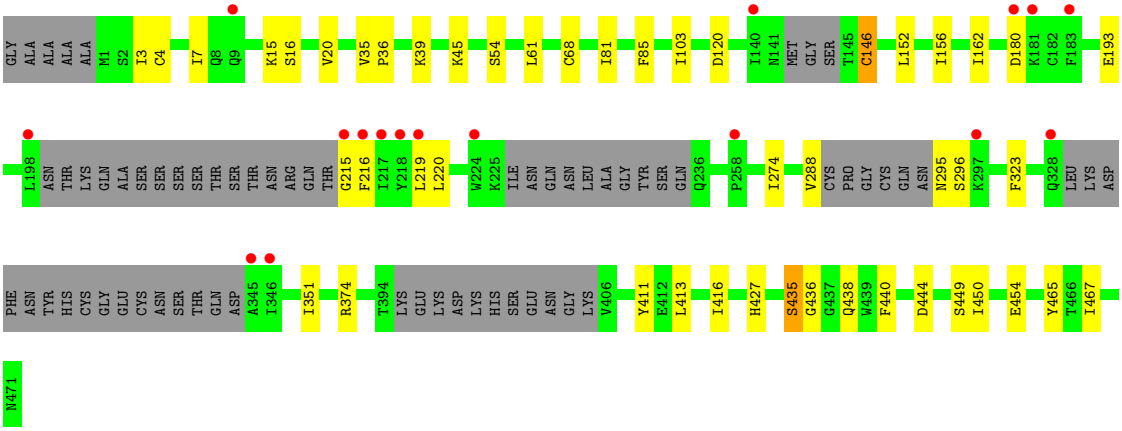




• Molecule 1: Ubiquitin carboxyl-terminal hydrolase

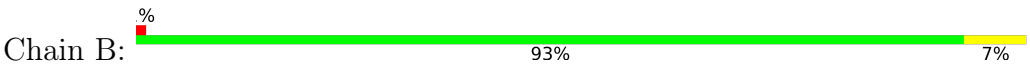
Chain D:

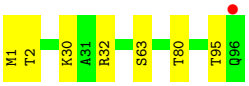




• Molecule 2: Transcription and mRNA export factor SUS1

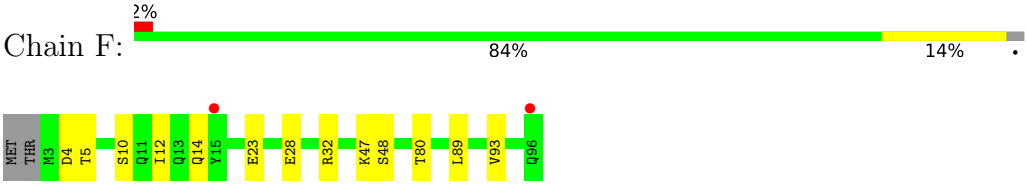
Chain B:





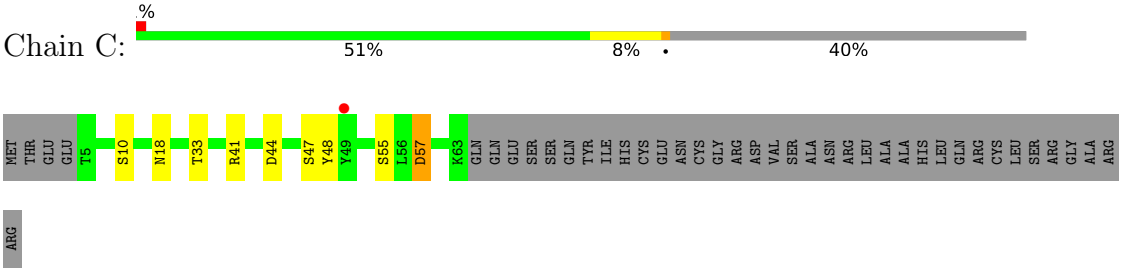
• Molecule 2: Transcription and mRNA export factor SUS1

Chain F:



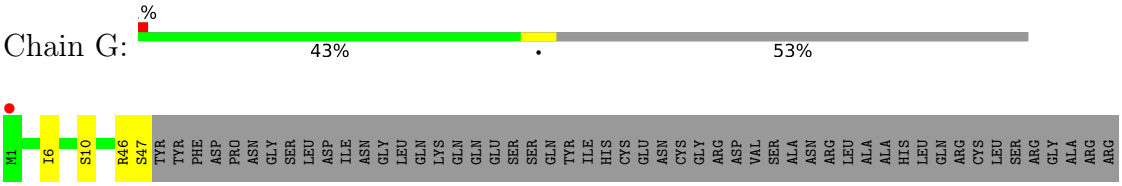
• Molecule 3: SAGA-associated factor 11

Chain C:



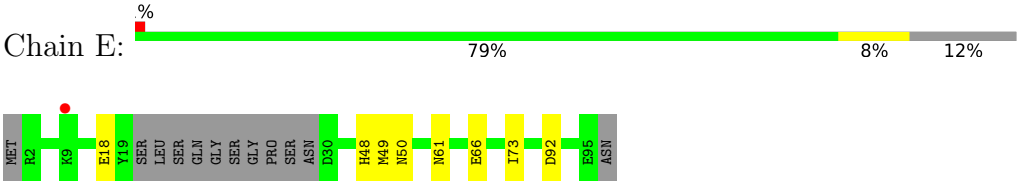
• Molecule 3: SAGA-associated factor 11

Chain G:



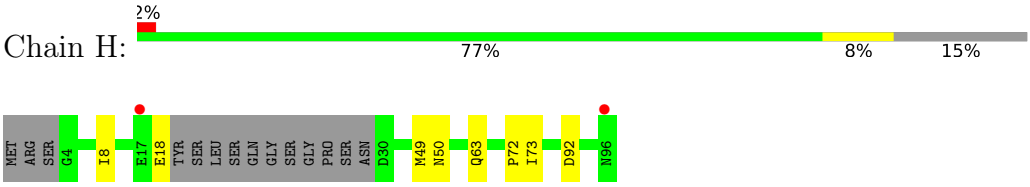
• Molecule 4: SAGA-associated factor 73

Chain E:



• Molecule 4: SAGA-associated factor 73

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.74Å 67.27Å 137.15Å 90.00° 106.84° 90.00°	Depositor
Resolution (Å)	47.02 – 2.80 46.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.02-2.80) 99.8 (46.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX	Depositor
R, R_{free}	0.182 , 0.241 0.184 , 0.237	Depositor DCC
R_{free} test set	1755 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	0/3612	0.66	0/4868
1	D	0.57	0/3370	0.67	0/4536
2	B	0.56	0/789	0.71	0/1062
2	F	0.56	0/774	0.69	0/1042
3	C	0.49	0/476	0.64	0/647
3	G	0.53	0/375	0.68	0/509
4	E	0.49	0/681	0.68	0/916
4	H	0.56	0/660	0.68	0/887
All	All	0.54	0/10737	0.67	0/14467

There are no bond length outliers.

There are no bond angle outliers.

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	3526	0	3459	30	1
1	D	3294	0	3251	33	0
2	B	780	0	792	5	0
2	F	765	0	773	12	1
3	C	471	0	478	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	374	0	390	5	0
4	E	669	0	671	7	0
4	H	649	0	650	9	0
5	A	6	0	0	0	0
5	D	5	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
6	A	8	0	0	1	0
6	B	5	0	0	1	0
6	D	25	0	0	0	0
6	E	3	0	0	1	0
6	F	4	0	0	1	0
6	G	2	0	0	1	0
6	H	6	0	0	0	0
All	All	10594	0	10464	86	1

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 4.

All (86) 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)
1:A:104:GLY:HA3	3:C:33:THR:HG23	1.73	0.71
4:E:66:GLU:HA	6:E:203:HOH:O	1.89	0.70
1:D:7[B]:ILE:HG23	1:D:85:PHE:CE1	2.30	0.67
1:D:193:GLU:OE2	1:D:215:GLY:N	2.28	0.67
2:F:5:THR:HG22	3:G:6:ILE:HG12	1.76	0.66
1:D:7[B]:ILE:HG23	1:D:85:PHE:CZ	2.34	0.62
1:D:295:ASN:N	1:D:296:SER:HA	2.14	0.61
1:A:53:ASN:O	3:C:18:ASN:HB3	2.01	0.61
4:E:18:GLU:N	4:E:18:GLU:CD	2.54	0.60
1:A:225:LYS:O	1:A:226:ILE:HD13	2.01	0.60
2:B:63:SER:OG	1:D:374:ARG:NH2	2.31	0.60
2:B:1:MET:N	6:B:101:HOH:O	2.35	0.59
1:A:447:VAL:O	3:C:57:ASP:HB2	2.02	0.59
3:G:47:SER:C	6:G:102:HOH:O	2.41	0.58
1:A:262[A]:GLU:OE1	1:A:265:ARG:NH1	2.37	0.58
1:A:253:TYR:O	1:A:257[B]:LEU:HD13	2.03	0.57
1:A:254:VAL:HA	1:A:257[B]:LEU:HD22	1.85	0.57
1:A:156:ILE:O	1:A:162:ILE:HD11	2.05	0.56
1:A:294:ASN:HD22	1:A:338:GLU:HB2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ILE:O	1:D:162:ILE:HD11	2.06	0.55
1:D:438:GLN:HG3	1:D:440:PHE:CE1	2.42	0.54
1:A:141:ASN:O	1:A:145:THR:OG1	2.24	0.54
2:B:30:LYS:NZ	4:E:48:HIS:HB3	2.24	0.53
1:A:156:ILE:O	1:A:156:ILE:HD12	2.09	0.53
1:D:156:ILE:O	1:D:156:ILE:HD12	2.09	0.52
1:D:413:LEU:HD21	1:D:416:ILE:HD11	1.91	0.52
1:A:467:ILE:HG13	4:E:49:MET:CE	2.39	0.52
1:D:146:CYS:SG	1:D:427:HIS:CD2	3.04	0.51
1:D:438:GLN:NE2	1:D:449:SER:OG	2.44	0.51
1:A:74:PHE:CD1	1:A:97:PHE:CE1	2.99	0.51
1:D:35:VAL:O	1:D:36:PRO:C	2.50	0.50
2:F:93:VAL:CG1	4:H:8:ILE:HG23	2.41	0.50
1:A:413:LEU:HD21	1:A:416[A]:ILE:HD11	1.92	0.50
2:F:93:VAL:HG13	4:H:8:ILE:HG23	1.93	0.50
2:F:32:ARG:NH2	2:F:80:THR:HG21	2.27	0.49
1:D:146:CYS:HB3	1:D:427:HIS:CE1	2.48	0.48
2:B:32:ARG:NH2	2:B:80:THR:HG21	2.29	0.47
1:A:141:ASN:OD1	1:A:141:ASN:N	2.48	0.46
2:B:30:LYS:HZ1	4:E:48:HIS:HB3	1.78	0.46
1:D:274:ILE:CD1	4:H:63:GLN:HE22	2.28	0.46
1:D:274:ILE:HD12	4:H:63:GLN:NE2	2.30	0.46
2:F:23:GLU:HG3	6:F:101:HOH:O	2.17	0.45
2:F:32:ARG:CZ	2:F:80:THR:HG21	2.47	0.45
1:D:467:ILE:HG13	4:H:49:MET:CE	2.47	0.45
1:A:54:SER:HB3	1:A:68:CYS:HB2	1.98	0.45
1:A:272:GLU:HG2	4:E:61:ASN:HD22	1.81	0.45
1:A:3:ILE:O	1:A:4:CYS:C	2.55	0.44
4:E:50:ASN:OD1	4:E:50:ASN:C	2.55	0.44
1:D:180:ASP:OD1	1:D:180:ASP:N	2.49	0.44
1:D:216:PHE:O	1:D:220:LEU:HD12	2.17	0.44
1:A:149:SER:HB3	6:A:604:HOH:O	2.18	0.44
1:D:3:ILE:O	1:D:4:CYS:C	2.56	0.44
1:A:169:ILE:O	1:A:173:ASN:ND2	2.45	0.43
1:D:20:VAL:HG13	1:D:61:LEU:HD21	2.00	0.43
1:D:288:VAL:HA	1:D:295:ASN:N	2.33	0.43
1:D:450:ILE:HG13	1:D:454:GLU:OE1	2.19	0.43
4:H:50:ASN:OD1	4:H:50:ASN:C	2.57	0.43
1:A:20:VAL:HG13	1:A:61:LEU:HD21	2.00	0.43
1:D:81:ILE:HG22	1:D:81:ILE:O	2.19	0.43
1:D:435:SER:HB3	4:H:72:PRO:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD12	3:C:48:TYR:CE1	2.54	0.42
3:G:46:ARG:HD3	3:G:46:ARG:HA	1.90	0.42
3:C:44:ASP:OD1	3:C:44:ASP:N	2.41	0.42
1:D:54:SER:HB3	1:D:68:CYS:HB2	2.00	0.42
1:D:4:CYS:O	1:D:7[B]:ILE:HD12	2.19	0.42
1:D:427:HIS:HE1	1:D:444:ASP:OD1	2.02	0.42
4:H:18:GLU:N	4:H:18:GLU:OE1	2.53	0.42
1:A:81:ILE:O	1:A:81:ILE:HG22	2.19	0.42
1:D:45:LYS:NZ	2:F:14:GLN:OE1	2.53	0.42
1:D:436:GLY:O	2:F:47:LYS:NZ	2.48	0.41
1:A:416[B]:ILE:HG23	1:A:431:PHE:HB2	2.03	0.41
3:C:57:ASP:OD1	3:C:57:ASP:C	2.59	0.41
1:A:107:ASP:OD1	3:C:41:ARG:NH2	2.54	0.41
1:D:7[B]:ILE:HG12	1:D:103:ILE:HD13	2.03	0.41
1:D:152:LEU:HD11	1:D:219:LEU:CD2	2.51	0.41
2:F:12[A]:ILE:HG21	2:F:89:LEU:CD2	2.51	0.41
1:A:139:LEU:HA	1:A:213:GLN:HE22	1.86	0.41
2:F:12[B]:ILE:HD13	2:F:89:LEU:HD22	2.03	0.41
1:A:152:LEU:HD11	1:A:219:LEU:CD2	2.51	0.41
2:F:5:THR:HG22	3:G:6:ILE:CG1	2.47	0.41
1:A:332:PHE:HA	1:A:333:ASN:HA	1.88	0.40
1:A:411:TYR:HB3	1:A:465:TYR:HB3	2.03	0.40
1:D:435:SER:CB	4:H:72:PRO:HA	2.51	0.40
1:D:411:TYR:HB3	1:D:465:TYR:HB3	2.03	0.40
1:A:61:LEU:HD12	1:A:61:LEU:HA	1.97	0.40
2:F:5:THR:CG2	3:G:6:ILE:HG12	2.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:OG	2:F:4:ASP:OD2[2_556]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/476 (91%)	406 (94%)	28 (6%)	0	100	100
1	D	397/476 (83%)	380 (96%)	17 (4%)	0	100	100
2	B	95/96 (99%)	95 (100%)	0	0	100	100
2	F	93/96 (97%)	93 (100%)	0	0	100	100
3	C	57/99 (58%)	55 (96%)	2 (4%)	0	100	100
3	G	45/99 (46%)	44 (98%)	1 (2%)	0	100	100
4	E	80/96 (83%)	76 (95%)	4 (5%)	0	100	100
4	H	78/96 (81%)	76 (97%)	2 (3%)	0	100	100
All	All	1279/1534 (83%)	1225 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	403/429 (94%)	390 (97%)	13 (3%)	39	73
1	D	376/429 (88%)	368 (98%)	8 (2%)	53	84
2	B	92/91 (101%)	90 (98%)	2 (2%)	52	83
2	F	90/91 (99%)	87 (97%)	3 (3%)	38	72
3	C	55/89 (62%)	51 (93%)	4 (7%)	14	38
3	G	45/89 (51%)	44 (98%)	1 (2%)	52	83
4	E	75/85 (88%)	73 (97%)	2 (3%)	44	78
4	H	73/85 (86%)	71 (97%)	2 (3%)	44	78
All	All	1209/1388 (87%)	1174 (97%)	35 (3%)	43	76

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	16	SER
1	A	39	LYS
1	A	120	ASP
1	A	140	ILE
1	A	146	CYS
1	A	262[A]	GLU
1	A	262[B]	GLU
1	A	322	SER
1	A	323	PHE
1	A	334	TYR
1	A	342	THR
1	A	351	ILE
2	B	2	THR
2	B	95	THR
3	C	10	SER
3	C	47	SER
3	C	55	SER
3	C	57	ASP
4	E	73	ILE
4	E	92	ASP
1	D	15	LYS
1	D	16	SER
1	D	39	LYS
1	D	120	ASP
1	D	146	CYS
1	D	323	PHE
1	D	351	ILE
1	D	435	SER
2	F	10	SER
2	F	28	GLU
2	F	48	SER
3	G	10	SER
4	H	73	ILE
4	H	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	164	HIS
1	D	268	ASN
1	D	427	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	438	GLN
1	D	452	GLN
1	D	459	GLN
3	G	34	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 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

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, 95^{th} 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	438/476 (92%)	0.20	20 (4%)	32	22	47, 80, 121, 149	0
1	D	409/476 (85%)	0.03	17 (4%)	36	26	44, 69, 114, 151	1 (0%)
2	B	96/96 (100%)	-0.04	1 (1%)	82	77	54, 70, 90, 113	0
2	F	94/96 (97%)	-0.11	2 (2%)	63	54	52, 67, 91, 110	0
3	C	59/99 (59%)	0.13	1 (1%)	70	63	49, 75, 126, 132	0
3	G	47/99 (47%)	-0.25	1 (2%)	63	54	46, 63, 91, 92	0
4	E	84/96 (87%)	0.18	1 (1%)	79	73	64, 83, 111, 121	0
4	H	82/96 (85%)	-0.08	2 (2%)	59	49	51, 70, 94, 112	0
All	All	1309/1534 (85%)	0.07	45 (3%)	45	35	44, 74, 115, 151	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TRP	6.6
1	A	216	PHE	5.0
1	D	198	LEU	4.6
1	A	218	TYR	4.6
1	D	216	PHE	4.5
1	A	367	HIS	4.3
1	D	218	TYR	4.1
1	D	217	ILE	4.1
1	A	373	ASN	4.1
1	A	368	LEU	3.7
1	D	215	GLY	3.6
2	F	15	TYR	3.5
1	D	140	ILE	3.4
1	D	258	PRO	3.3
1	D	345	ALA	3.3
2	B	96	GLN	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	224	TRP	3.2
1	D	346	ILE	3.2
1	A	217	ILE	3.1
1	A	226	ILE	3.1
1	A	213	GLN	3.1
2	F	96	GLN	3.0
1	A	374	ARG	2.9
1	D	297	LYS	2.9
1	A	424	ASN	2.9
1	A	288	VAL	2.9
1	A	198	LEU	2.7
1	D	328	GLN	2.7
1	A	15	LYS	2.5
1	A	366	GLU	2.5
4	E	9	LYS	2.4
3	G	1	MET	2.4
3	C	49	TYR	2.3
1	D	183	PHE	2.3
1	D	9	GLN	2.3
1	A	369	LEU	2.2
1	A	122	CYS	2.2
4	H	96	ASN	2.2
1	A	423	VAL	2.2
4	H	17	GLU	2.1
1	D	219	LEU	2.1
1	D	181	LYS	2.1
1	A	140	ILE	2.0
1	D	180	ASP	2.0
1	A	138	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	506	1/1	0.98	0.05	115,115,115,115	0
5	ZN	E	101	1/1	0.98	0.13	102,102,102,102	0
5	ZN	A	505	1/1	0.99	0.13	90,90,90,90	0
5	ZN	A	501	1/1	0.99	0.15	73,73,73,73	0
5	ZN	A	503	1/1	0.99	0.15	76,76,76,76	0
5	ZN	D	501	1/1	0.99	0.10	75,75,75,75	0
5	ZN	D	502	1/1	0.99	0.11	80,80,80,80	0
5	ZN	H	101	1/1	0.99	0.12	73,73,73,73	0
5	ZN	A	502	1/1	1.00	0.18	55,55,55,55	0
5	ZN	D	503	1/1	1.00	0.14	58,58,58,58	0
5	ZN	D	504	1/1	1.00	0.15	64,64,64,64	0
5	ZN	D	505	1/1	1.00	0.16	70,70,70,70	0
5	ZN	A	504	1/1	1.00	0.18	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.