



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:00 AM UTC

PDB ID : 5K1A / pdb_00005k1a
Title : Crystal structure of the UAF1-USP12 complex in C2 space group
Authors : Li, H.; D'Andrea, A.D.; Zheng, N.
Deposited on : 2016-05-18
Resolution : 2.30 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

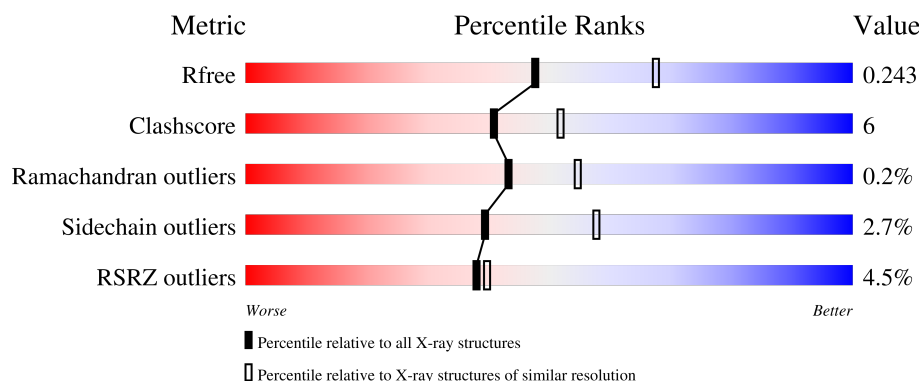
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

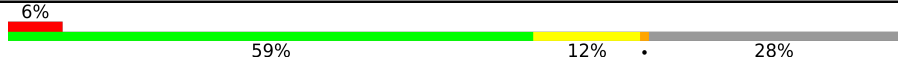
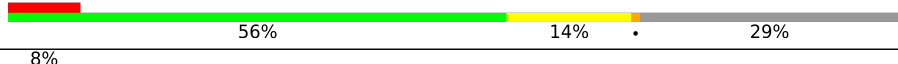
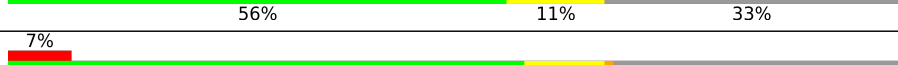
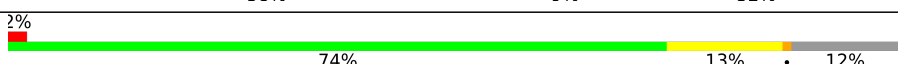
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	331	
1	C	331	
1	E	331	
1	G	331	
2	B	677	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	677	2% 75% 12% • 12%
2	F	677	% 74% 13% • 11%
2	H	677	2% 75% 11% • 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27654 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 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1886	1217	310	345	14			
1	C	236	Total	C	N	O	S	0	0	0
			1882	1215	308	345	14			
1	E	222	Total	C	N	O	S	0	0	0
			1747	1131	285	317	14			
1	G	224	Total	C	N	O	S	0	1	0
			1768	1136	290	328	14			

- Molecule 2 is a protein called WD repeat-containing protein 48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	595	Total	C	N	O	S	0	0	0
			4690	2973	818	872	27			
2	D	597	Total	C	N	O	S	0	0	0
			4701	2976	822	876	27			
2	F	600	Total	C	N	O	S	0	0	0
			4731	2994	825	885	27			
2	H	594	Total	C	N	O	S	0	0	0
			4664	2948	819	870	27			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

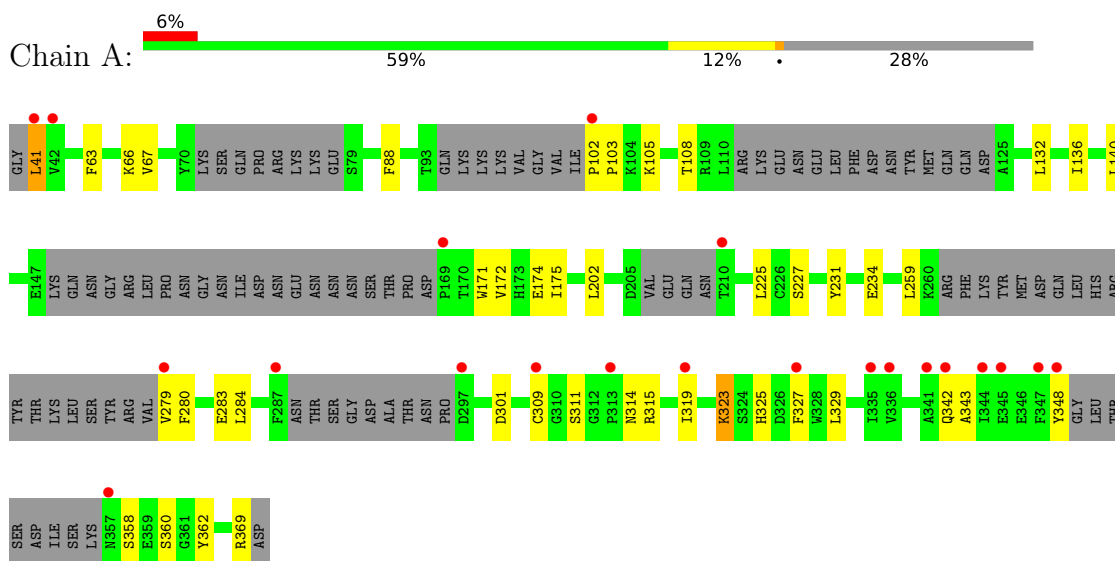
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total 81	O 81	0	0
4	B	286	Total 286	O 286	0	0
4	C	82	Total 82	O 82	0	0
4	D	334	Total 334	O 334	0	0
4	E	68	Total 68	O 68	0	0
4	F	364	Total 364	O 364	0	0
4	G	57	Total 57	O 57	0	0
4	H	309	Total 309	O 309	0	0

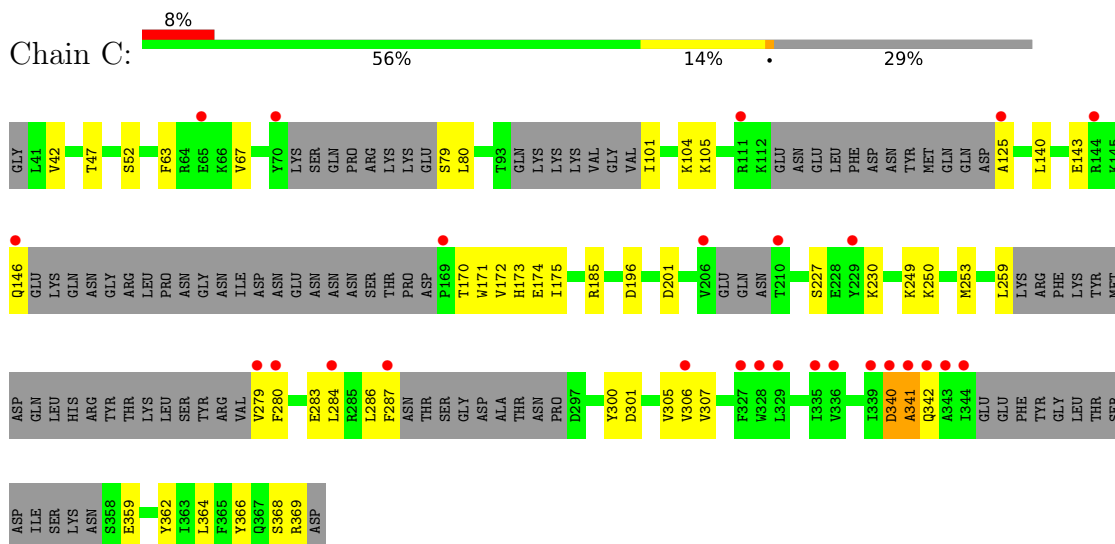
3 Residue-property plots [i](#)

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 12

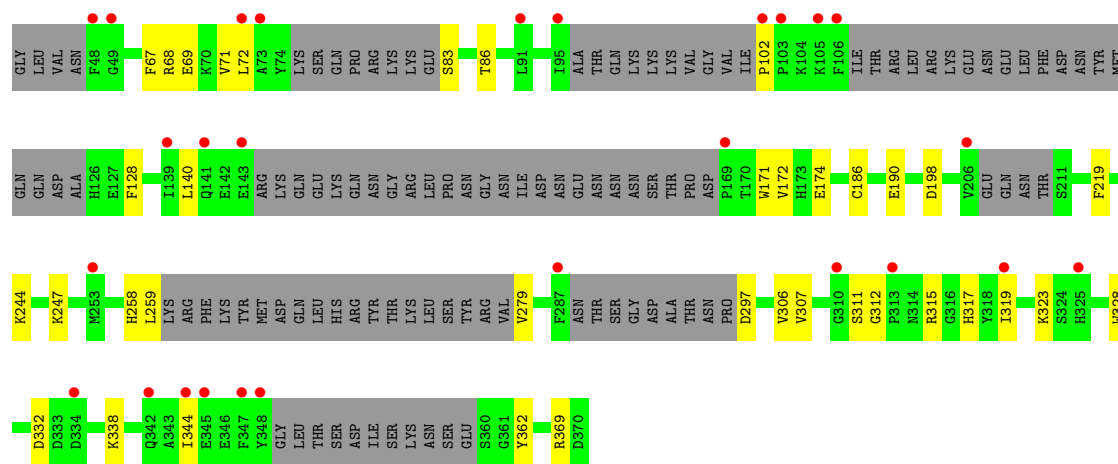


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12

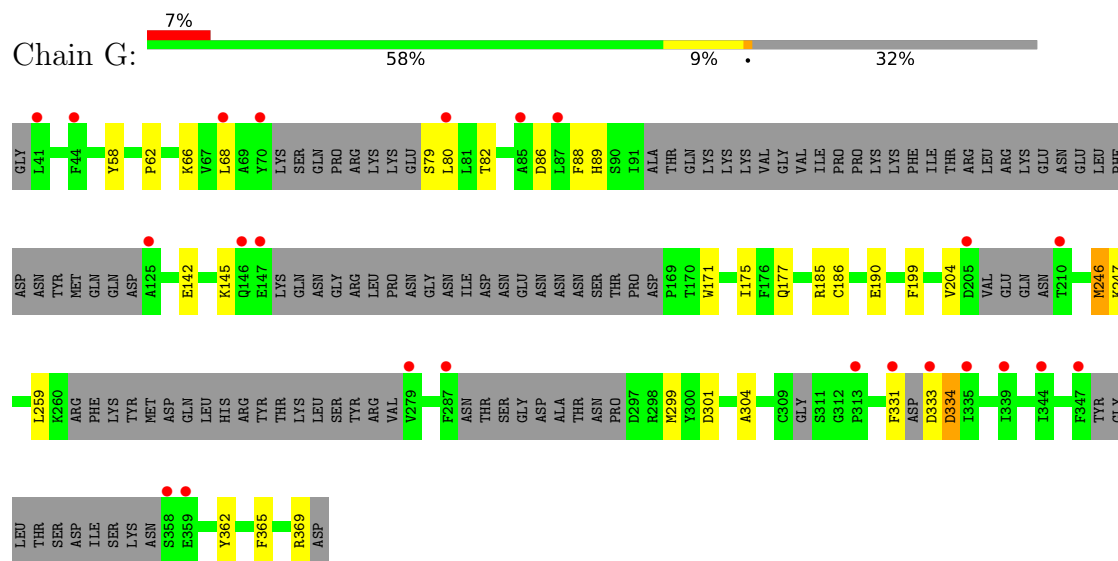


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12

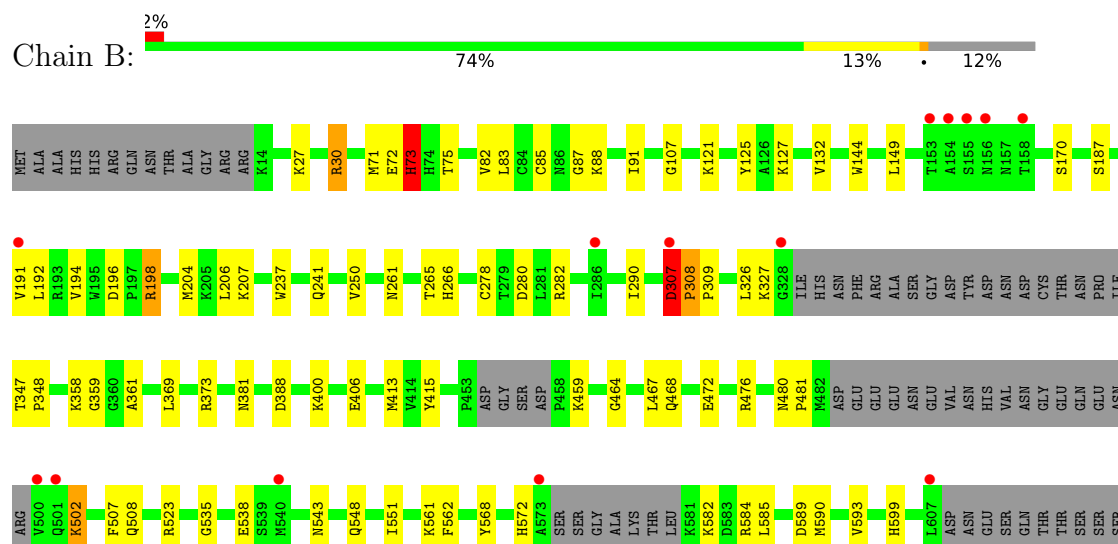




• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 12

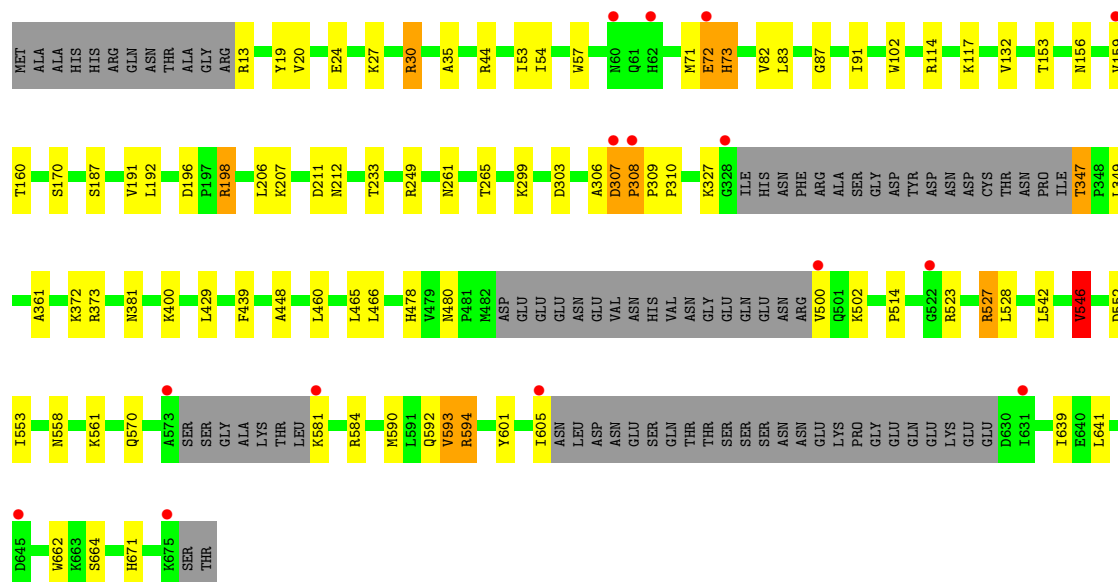
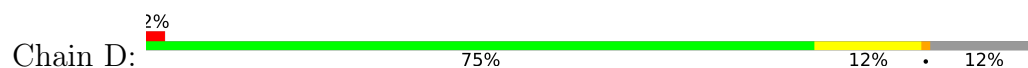


• Molecule 2: WD repeat-containing protein 48

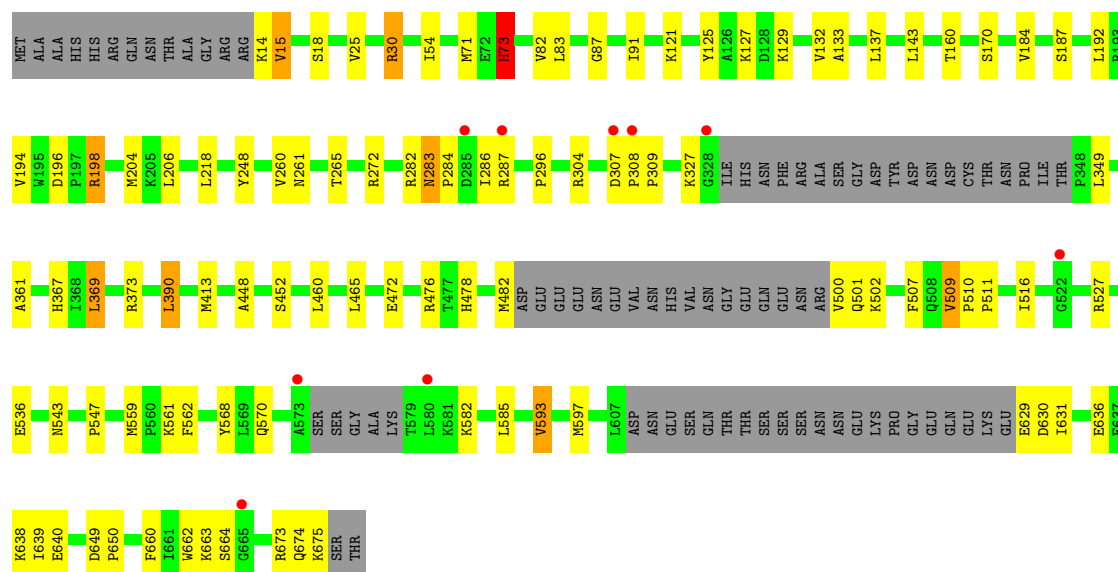
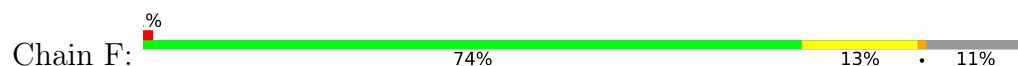




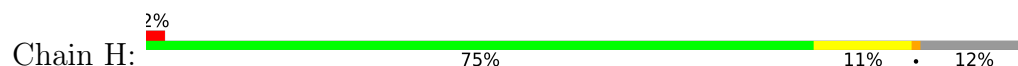
• Molecule 2: WD repeat-containing protein 48

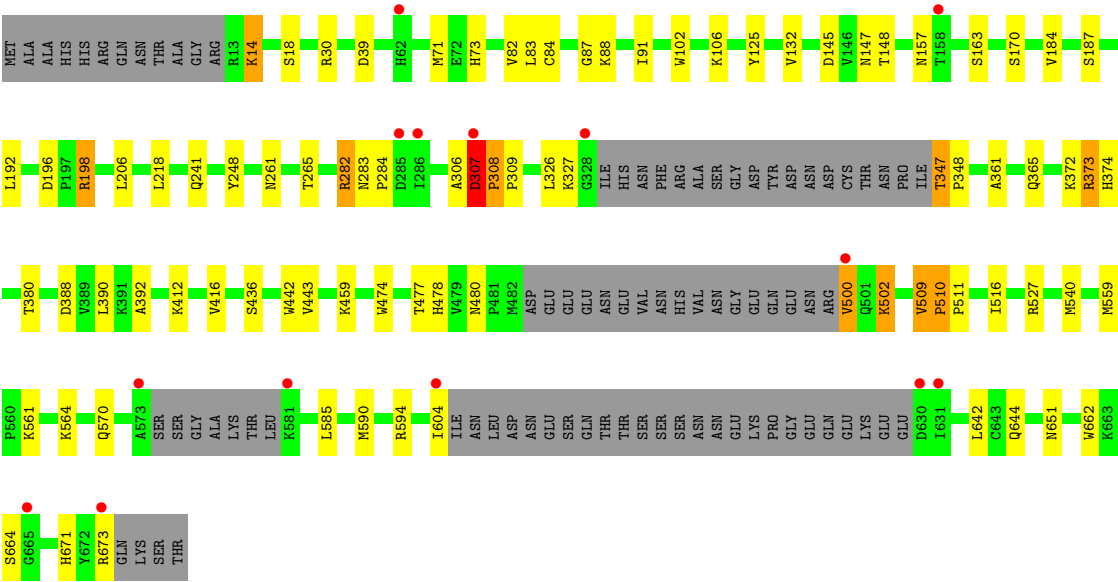


• Molecule 2: WD repeat-containing protein 48



• Molecule 2: WD repeat-containing protein 48





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	262.43Å 103.30Å 178.47Å 90.00° 117.47° 90.00°	Depositor
Resolution (Å)	49.10 – 2.30 49.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.10-2.30) 93.0 (49.10-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_1760	Depositor
R, R_{free}	0.188 , 0.239 0.194 , 0.243	Depositor DCC
R_{free} test set	9518 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	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	0.95	EDS
Total number of atoms	27654	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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	0.54	0/1923	0.84	5/2601 (0.2%)
1	C	0.56	2/1918 (0.1%)	0.95	6/2591 (0.2%)
1	E	0.51	0/1782	0.90	5/2408 (0.2%)
1	G	0.52	0/1803	0.81	0/2435
2	B	0.67	3/4783 (0.1%)	0.89	10/6485 (0.2%)
2	D	0.68	5/4795 (0.1%)	0.88	14/6502 (0.2%)
2	F	0.67	3/4825 (0.1%)	0.88	15/6543 (0.2%)
2	H	0.68	4/4757 (0.1%)	0.89	12/6452 (0.2%)
All	All	0.64	17/26586 (0.1%)	0.88	67/36017 (0.2%)

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
1	A	0	1
2	B	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	307	ASP	CA-C	-8.37	1.42	1.52
2	D	307	ASP	C-N	7.64	1.42	1.33
2	H	307	ASP	C-N	7.29	1.42	1.33
2	B	307	ASP	C-N	7.29	1.42	1.33
2	F	307	ASP	C-N	6.64	1.41	1.33
2	D	307	ASP	CA-C	-6.24	1.45	1.52
2	F	308	PRO	C-N	6.20	1.40	1.33
2	D	308	PRO	C-N	6.15	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	PRO	C-N	6.04	1.40	1.33
2	H	308	PRO	C-N	5.84	1.40	1.33
2	D	73	HIS	CA-C	5.71	1.60	1.52
1	C	340	ASP	C-O	-5.35	1.17	1.23
2	B	309	PRO	N-CD	5.15	1.54	1.47
2	H	309	PRO	C-O	-5.15	1.18	1.24
1	C	340	ASP	C-N	-5.09	1.27	1.33
2	D	309	PRO	N-CD	5.07	1.54	1.47
2	F	309	PRO	N-CD	5.04	1.54	1.47

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	ASP	O-C-N	-16.97	100.37	123.11
2	B	72	GLU	N-CA-C	13.52	129.90	113.41
2	F	73	HIS	N-CA-CB	11.08	129.21	110.49
2	D	73	HIS	N-CA-C	10.61	127.19	114.04
2	B	73	HIS	N-CA-C	10.17	132.47	110.80
1	A	343	ALA	N-CA-C	-9.80	101.08	113.23
1	E	344	ILE	N-CA-C	9.46	120.07	110.23
1	C	341	ALA	CA-C-N	-9.43	106.68	120.82
1	C	341	ALA	C-N-CA	-9.43	106.68	120.82
1	E	102	PRO	CA-C-N	-8.53	109.18	119.84
1	E	102	PRO	C-N-CA	-8.53	109.18	119.84
2	F	307	ASP	CA-C-N	-8.30	111.83	120.38
2	F	307	ASP	C-N-CA	-8.30	111.83	120.38
2	D	307	ASP	CA-C-N	-8.21	111.93	120.38
2	D	307	ASP	C-N-CA	-8.21	111.93	120.38
2	B	307	ASP	CA-C-N	-8.05	112.09	120.38
2	B	307	ASP	C-N-CA	-8.05	112.09	120.38
2	H	307	ASP	CA-C-N	-8.03	112.11	120.38
2	H	307	ASP	C-N-CA	-8.03	112.11	120.38
1	C	341	ALA	O-C-N	7.96	132.74	122.39
1	E	344	ILE	CB-CA-C	-7.36	102.28	111.70
2	F	308	PRO	CA-C-N	-7.17	113.00	120.38
2	F	308	PRO	C-N-CA	-7.17	113.00	120.38
2	B	308	PRO	CA-C-N	-6.99	113.19	120.38
2	B	308	PRO	C-N-CA	-6.99	113.19	120.38
2	H	308	PRO	CA-C-N	-6.97	113.20	120.38
2	H	308	PRO	C-N-CA	-6.97	113.20	120.38
2	H	283	ASN	CA-C-N	6.81	126.78	119.28
2	H	283	ASN	C-N-CA	6.81	126.78	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	308	PRO	N-CA-C	-6.67	102.56	110.70
2	H	347	THR	CA-C-N	6.64	126.68	119.90
2	H	347	THR	C-N-CA	6.64	126.68	119.90
2	D	308	PRO	CA-C-N	-6.57	113.61	120.38
2	D	308	PRO	C-N-CA	-6.57	113.61	120.38
2	B	662	TRP	N-CA-C	-6.22	100.96	110.30
2	D	72	GLU	N-CA-C	6.22	120.67	107.67
2	D	546	VAL	CA-C-N	6.19	126.38	120.31
2	D	546	VAL	C-N-CA	6.19	126.38	120.31
2	D	546	VAL	N-CA-CB	5.97	115.64	110.08
2	F	509	VAL	CA-C-N	-5.89	114.31	120.38
2	F	509	VAL	C-N-CA	-5.89	114.31	120.38
1	A	358	SER	N-CA-C	5.85	119.09	109.85
2	B	662	TRP	CB-CA-C	5.73	118.03	110.06
2	D	73	HIS	O-C-N	5.72	129.11	122.25
2	H	307	ASP	N-CA-C	-5.72	97.18	109.81
1	C	340	ASP	CA-C-N	5.71	129.73	120.60
1	C	340	ASP	C-N-CA	5.71	129.73	120.60
2	H	510	PRO	CA-C-N	5.71	125.83	119.32
2	H	510	PRO	C-N-CA	5.71	125.83	119.32
2	H	373	ARG	N-CA-C	-5.62	108.21	114.62
1	A	227	SER	CB-CA-C	-5.58	109.64	117.23
2	F	14	LYS	CA-C-N	-5.50	116.00	123.10
2	F	14	LYS	C-N-CA	-5.50	116.00	123.10
1	A	280	PHE	CA-C-N	5.40	125.82	119.99
1	A	280	PHE	C-N-CA	5.40	125.82	119.99
2	B	523	ARG	N-CA-C	5.31	116.91	108.67
2	F	639	ILE	N-CA-C	5.23	115.44	108.11
2	D	347	THR	CA-C-N	5.23	125.44	120.31
2	D	347	THR	C-N-CA	5.23	125.44	120.31
2	F	283	ASN	CA-C-N	5.21	124.93	119.82
2	F	283	ASN	C-N-CA	5.21	124.93	119.82
1	E	128	PHE	N-CA-C	5.18	116.93	111.28
2	B	308	PRO	N-CA-C	-5.15	104.41	110.70
2	F	452	SER	CA-C-N	5.08	125.08	119.90
2	F	452	SER	C-N-CA	5.08	125.08	119.90
2	D	72	GLU	CA-C-N	5.07	131.39	122.42
2	D	72	GLU	C-N-CA	5.07	131.39	122.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	GLN	Peptide
2	B	599	HIS	Sidechain

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	1886	0	1796	30	0
1	C	1882	0	1825	36	0
1	E	1747	0	1656	27	1
1	G	1768	0	1659	18	0
2	B	4690	0	4693	60	0
2	D	4701	0	4698	59	1
2	F	4731	0	4732	56	0
2	H	4664	0	4649	57	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	81	0	0	0	0
4	B	286	0	0	9	0
4	C	82	0	0	4	0
4	D	334	0	0	11	0
4	E	68	0	0	7	0
4	F	364	0	0	7	0
4	G	57	0	0	1	0
4	H	309	0	0	7	0
All	All	27654	0	25708	335	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 6.

All (335) 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:C:284:LEU:HD13	1:C:366:TYR:CE1	1.81	1.16
1:A:314:ASN:HB3	1:A:319:ILE:CD1	1.84	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASN:HB3	1:A:319:ILE:HD11	1.45	0.95
1:C:284:LEU:CD1	1:C:366:TYR:CE1	2.49	0.95
2:F:30:ARG:NH1	2:F:361:ALA:O	2.05	0.89
2:H:474:TRP:O	2:H:477:THR:OG1	1.88	0.88
1:A:314:ASN:HB3	1:A:319:ILE:HD13	1.56	0.87
2:B:241:GLN:OE1	4:B:701:HOH:O	1.92	0.86
2:H:30:ARG:NH1	2:H:361:ALA:O	2.10	0.85
1:C:284:LEU:HD11	1:C:366:TYR:CZ	2.14	0.83
1:A:314:ASN:CB	1:A:319:ILE:CD1	2.58	0.81
2:D:159:VAL:HG12	2:D:160:THR:O	1.79	0.81
1:A:309:CYS:SG	1:A:348:TYR:CD1	2.73	0.81
2:H:307:ASP:HB3	2:H:308:PRO:HD3	1.63	0.80
2:F:327:LYS:H	2:F:349:LEU:HD21	1.46	0.80
2:H:478:HIS:HB3	2:H:500:VAL:HG23	1.63	0.79
2:F:536:GLU:OE1	4:F:701:HOH:O	2.02	0.78
2:D:83:LEU:HD22	2:D:87:GLY:HA2	1.68	0.76
1:E:307:VAL:O	1:E:319:ILE:HG12	1.86	0.76
1:C:284:LEU:CD1	1:C:366:TYR:CZ	2.69	0.75
2:D:592:GLN:OE1	2:D:594:ARG:NH1	2.20	0.75
2:H:594:ARG:NH2	2:H:651:ASN:OD1	2.21	0.73
1:A:309:CYS:SG	1:A:348:TYR:HD1	2.12	0.73
2:D:117:LYS:HD3	2:D:523:ARG:HH21	1.53	0.72
1:A:309:CYS:SG	1:A:348:TYR:CE1	2.83	0.72
1:E:198:ASP:O	4:E:501:HOH:O	2.08	0.72
1:G:86:ASP:HA	1:G:89:HIS:CE1	2.24	0.72
1:C:104:LYS:O	1:C:104:LYS:HG2	1.90	0.71
1:E:315:ARG:HH11	1:E:315:ARG:HG3	1.53	0.71
1:A:314:ASN:CB	1:A:319:ILE:HD13	2.20	0.70
1:C:101:ILE:N	4:C:503:HOH:O	2.23	0.70
2:H:170:SER:O	2:H:187:SER:HB2	1.92	0.70
1:E:297:ASP:O	4:E:502:HOH:O	2.09	0.70
2:B:388:ASP:OD2	4:B:702:HOH:O	2.09	0.69
2:B:373:ARG:NH1	2:B:388:ASP:OD1	2.25	0.69
2:B:406:GLU:OE1	4:B:703:HOH:O	2.10	0.69
1:A:314:ASN:O	1:A:319:ILE:HD11	1.93	0.68
2:D:307:ASP:HB3	2:D:308:PRO:CD	2.23	0.68
2:F:373:ARG:NH2	2:F:448:ALA:O	2.27	0.68
2:H:459:LYS:HD2	2:H:459:LYS:N	2.09	0.68
1:C:284:LEU:HD13	1:C:366:TYR:CD1	2.29	0.68
1:E:297:ASP:N	4:E:504:HOH:O	2.27	0.67
2:B:307:ASP:HB3	2:B:308:PRO:CD	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:673:ARG:NH2	4:F:708:HOH:O	2.26	0.67
1:E:258:HIS:ND1	4:E:506:HOH:O	2.28	0.67
2:H:241:GLN:NE2	4:H:703:HOH:O	2.28	0.65
2:D:159:VAL:HG12	2:D:160:THR:N	2.09	0.65
2:B:415:TYR:HD2	2:B:655:ARG:HG2	1.61	0.65
2:D:523:ARG:NH1	4:D:704:HOH:O	2.30	0.65
1:C:125:ALA:N	4:C:506:HOH:O	2.29	0.65
1:E:171:TRP:HA	1:E:174:GLU:HG2	1.79	0.64
1:A:314:ASN:CB	1:A:319:ILE:HD11	2.23	0.64
2:B:30:ARG:NH1	4:B:709:HOH:O	2.32	0.63
1:E:307:VAL:HG23	1:E:319:ILE:CG1	2.29	0.63
1:G:79:SER:O	1:G:82:THR:OG1	2.15	0.63
2:H:442:TRP:HH2	2:H:559:MET:HE3	1.63	0.62
1:A:140:LEU:HD12	1:A:172:VAL:HG23	1.81	0.62
2:H:192:LEU:HB2	2:H:206:LEU:HB2	1.83	0.61
2:F:91:ILE:HD13	2:F:132:VAL:HG21	1.81	0.61
1:G:185:ARG:NH1	4:G:501:HOH:O	2.17	0.61
2:H:373:ARG:NH1	2:H:390:LEU:HB3	2.16	0.61
2:D:53:ILE:HG12	2:D:72:GLU:HG2	1.82	0.60
2:D:327:LYS:H	2:D:349:LEU:HD21	1.65	0.60
1:E:311:SER:O	4:E:503:HOH:O	2.16	0.60
2:D:13:ARG:N	4:D:708:HOH:O	2.33	0.60
2:D:153:THR:HG23	2:D:156:ASN:H	1.67	0.60
2:B:30:ARG:NH1	2:B:361:ALA:O	2.35	0.59
2:F:127:LYS:NZ	4:F:716:HOH:O	2.36	0.59
2:B:507:PHE:O	4:B:704:HOH:O	2.16	0.59
1:E:315:ARG:HG3	1:E:315:ARG:NH1	2.16	0.59
2:B:83:LEU:HD22	2:B:87:GLY:HA2	1.85	0.59
2:B:373:ARG:HD2	4:B:940:HOH:O	2.01	0.59
2:D:114:ARG:NH2	4:D:703:HOH:O	2.29	0.59
2:F:248:TYR:CD1	2:F:284:PRO:HB3	2.37	0.59
2:F:476:ARG:NH1	2:F:543:ASN:OD1	2.35	0.59
2:F:248:TYR:HD1	2:F:284:PRO:HB3	1.68	0.59
2:H:196:ASP:OD1	2:H:198:ARG:HD3	2.03	0.58
2:B:373:ARG:HG2	2:B:373:ARG:HH11	1.69	0.58
2:F:18:SER:HB2	2:F:516:ILE:HB	1.85	0.58
1:C:52:SER:HB3	1:C:306:VAL:HG13	1.84	0.58
2:F:82:VAL:HG11	2:F:125:TYR:HB2	1.85	0.58
1:C:301:ASP:OD2	1:C:369:ARG:HD3	2.04	0.58
1:G:62:PRO:HB2	1:G:175:ILE:HD12	1.86	0.58
2:H:91:ILE:HD13	2:H:132:VAL:HG21	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:283:ASN:HB3	2:F:286:ILE:HD13	1.86	0.57
1:C:104:LYS:HG3	4:C:572:HOH:O	2.04	0.57
2:D:170:SER:O	2:D:187:SER:HB2	2.03	0.57
1:C:341:ALA:O	1:C:342:GLN:C	2.47	0.57
2:B:170:SER:O	2:B:187:SER:HB2	2.04	0.57
2:D:478:HIS:CD2	2:D:502:LYS:HG3	2.40	0.57
2:B:307:ASP:HB3	2:B:308:PRO:HD3	1.87	0.57
1:E:307:VAL:HG23	1:E:319:ILE:HD11	1.85	0.57
2:F:662:TRP:CH2	2:F:664:SER:HB2	2.40	0.57
2:H:307:ASP:HB3	2:H:308:PRO:CD	2.32	0.57
2:D:91:ILE:HD13	2:D:132:VAL:HG21	1.87	0.56
2:B:280:ASP:OD1	2:B:282:ARG:HG3	2.05	0.56
1:A:259:LEU:HD12	1:A:362:TYR:CZ	2.40	0.56
2:B:476:ARG:NH1	2:B:543:ASN:OD1	2.38	0.56
2:B:191:VAL:HG22	2:B:207:LYS:HG3	1.87	0.56
2:F:500:VAL:N	4:F:721:HOH:O	2.38	0.56
1:G:304:ALA:HB3	1:G:365:PHE:HB2	1.88	0.56
2:H:306:ALA:O	2:H:307:ASP:C	2.49	0.56
2:D:159:VAL:CG1	2:D:160:THR:N	2.69	0.55
2:F:390:LEU:HD22	2:F:507:PHE:CZ	2.41	0.55
2:D:480:ASN:HB2	2:D:500:VAL:N	2.22	0.55
1:G:66:LYS:HG2	1:G:171:TRP:CD2	2.41	0.55
2:F:413:MET:HE2	2:F:660:PHE:HB3	1.87	0.55
1:G:331:PHE:C	1:G:333:ASP:N	2.65	0.55
2:H:261:ASN:HD21	2:H:265:THR:CG2	2.18	0.55
2:H:373:ARG:HH11	2:H:373:ARG:HG3	1.72	0.55
1:A:171:TRP:HA	1:A:174:GLU:HG2	1.89	0.55
2:D:480:ASN:HB3	2:F:585:LEU:HD23	1.89	0.55
1:C:175:ILE:HA	1:C:253:MET:HE3	1.88	0.54
2:B:629:GLU:HG2	2:B:630:ASP:H	1.70	0.54
2:D:373:ARG:NH1	2:D:448:ALA:O	2.39	0.54
1:E:259:LEU:HD12	1:E:362:TYR:CZ	2.42	0.54
2:F:501:GLN:OE1	4:F:703:HOH:O	2.18	0.54
2:F:638:LYS:HE2	2:F:674:GLN:OE1	2.06	0.54
2:D:71:MET:HB3	2:D:102:TRP:CZ3	2.42	0.54
1:E:83:SER:O	1:E:86:THR:OG1	2.21	0.54
1:E:140:LEU:HD11	1:E:171:TRP:CE2	2.42	0.54
2:F:663:LYS:NZ	4:F:720:HOH:O	2.40	0.54
2:D:593:VAL:HG13	2:D:641:LEU:HD12	1.89	0.54
1:G:68:LEU:HD22	1:G:89:HIS:HB3	1.90	0.54
2:H:642:LEU:HD21	2:H:673:ARG:HH21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:372:LYS:NZ	2:H:416:VAL:O	2.41	0.54
1:A:105:LYS:O	1:A:108:THR:OG1	2.24	0.53
2:B:265:THR:HG23	2:B:266:HIS:ND1	2.24	0.53
2:F:570:GLN:OE1	2:F:582:LYS:NZ	2.37	0.53
1:C:47:THR:OG1	2:F:160:THR:HG23	2.08	0.53
1:C:171:TRP:HA	1:C:174:GLU:HG2	1.91	0.53
2:D:30:ARG:NH1	2:D:361:ALA:O	2.42	0.52
2:F:272:ARG:HA	2:F:296:PRO:HB3	1.91	0.52
2:H:147:ASN:ND2	4:H:717:HOH:O	2.41	0.52
2:F:192:LEU:HB2	2:F:206:LEU:HB2	1.92	0.52
2:H:83:LEU:HD22	2:H:87:GLY:HA2	1.92	0.52
2:B:82:VAL:HG11	2:B:125:TYR:HB2	1.92	0.52
1:C:340:ASP:O	1:C:342:GLN:N	2.43	0.52
1:G:259:LEU:HD12	1:G:362:TYR:CE2	2.44	0.52
2:D:527:ARG:HD3	2:D:527:ARG:C	2.35	0.52
1:A:311:SER:HA	1:A:315:ARG:HD3	1.91	0.52
2:D:20:VAL:HB	2:D:514:PRO:HG2	1.92	0.52
2:D:347:THR:N	4:D:721:HOH:O	2.41	0.52
2:D:327:LYS:O	2:D:349:LEU:HD11	2.09	0.52
2:B:381:ASN:O	2:B:400:LYS:HE3	2.09	0.51
2:D:558:ASN:ND2	2:F:562:PHE:O	2.42	0.51
2:D:72:GLU:OE1	4:D:701:HOH:O	2.19	0.51
2:D:261:ASN:HD21	2:D:265:THR:CG2	2.23	0.51
2:F:472:GLU:HG2	2:F:502:LYS:HE2	1.92	0.51
2:H:374:HIS:NE2	4:H:709:HOH:O	2.34	0.51
2:D:584:ARG:NH1	4:D:723:HOH:O	2.42	0.51
2:B:280:ASP:OD1	2:B:282:ARG:CG	2.58	0.51
1:A:259:LEU:HD12	1:A:362:TYR:CE2	2.46	0.50
2:F:170:SER:O	2:F:187:SER:HB2	2.09	0.50
1:C:280:PHE:HD1	1:C:364:LEU:HD21	1.77	0.50
2:H:412:LYS:NZ	4:H:719:HOH:O	2.43	0.50
1:A:225:LEU:HD12	1:A:231:TYR:HB2	1.93	0.50
2:D:542:LEU:O	2:D:546:VAL:HG13	2.12	0.50
1:G:333:ASP:O	1:G:334:ASP:HB2	2.11	0.50
2:F:568:TYR:CD1	2:F:582:LYS:HE3	2.46	0.50
2:H:145:ASP:OD2	2:H:148:THR:HG23	2.12	0.50
2:D:114:ARG:NE	4:D:703:HOH:O	2.40	0.50
2:B:196:ASP:OD1	2:B:198:ARG:HD3	2.12	0.49
1:E:317:HIS:NE2	1:E:332:ASP:OD1	2.41	0.49
1:G:177:GLN:HA	1:G:199:PHE:O	2.12	0.49
2:H:18:SER:HB2	2:H:516:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:585:LEU:HD23	2:H:480:ASN:HB3	1.94	0.49
1:G:171:TRP:O	1:G:175:ILE:HG12	2.12	0.49
2:B:480:ASN:HB3	2:H:585:LEU:HD23	1.95	0.49
1:A:41:LEU:HA	2:H:157:ASN:HB2	1.94	0.49
1:E:323:LYS:HD3	1:E:328:TRP:CE2	2.47	0.49
2:H:478:HIS:CD2	2:H:502:LYS:HG2	2.47	0.49
1:A:132:LEU:O	1:A:136:ILE:HG13	2.13	0.49
2:D:196:ASP:OD1	2:D:198:ARG:HD3	2.13	0.49
1:C:300:TYR:CZ	1:C:368:SER:HB3	2.48	0.48
1:E:307:VAL:HG23	1:E:319:ILE:CD1	2.43	0.48
2:H:306:ALA:O	2:H:307:ASP:O	2.31	0.48
1:C:52:SER:CB	1:C:306:VAL:HG13	2.44	0.48
1:G:299:MET:HG2	1:G:369:ARG:NH2	2.27	0.48
1:C:52:SER:HB3	1:C:306:VAL:CG1	2.43	0.48
2:F:460:LEU:HB3	2:F:465:LEU:HD11	1.96	0.48
2:B:662:TRP:CZ2	2:B:664:SER:HB2	2.49	0.48
2:H:14:LYS:HB2	2:H:14:LYS:HE3	1.56	0.48
2:B:548:GLN:HA	2:B:551:ILE:HD12	1.96	0.48
1:C:280:PHE:CD1	1:C:364:LEU:HD21	2.49	0.47
2:B:278:CYS:HB2	2:B:290:ILE:HD11	1.95	0.47
2:F:559:MET:HA	2:F:559:MET:HE2	1.95	0.47
1:E:312:GLY:O	1:E:315:ARG:HD3	2.14	0.47
1:A:327:PHE:HE1	1:A:329:LEU:HD21	1.79	0.47
2:H:392:ALA:HB3	2:H:509:VAL:HG22	1.97	0.47
1:A:283:GLU:OE2	1:A:369:ARG:NH2	2.40	0.47
1:A:309:CYS:SG	1:A:348:TYR:HE1	2.34	0.47
2:D:570:GLN:O	2:D:671:HIS:HA	2.15	0.47
2:F:196:ASP:OD1	2:F:198:ARG:HD3	2.14	0.47
2:H:261:ASN:HD21	2:H:265:THR:HG22	1.78	0.47
2:H:570:GLN:O	2:H:671:HIS:HA	2.13	0.47
1:A:140:LEU:HD11	1:A:171:TRP:CE2	2.49	0.47
1:G:58:TYR:HA	1:G:88:PHE:CE2	2.50	0.47
2:F:597:MET:CE	2:F:636:GLU:HA	2.45	0.47
2:D:460:LEU:HD13	2:D:465:LEU:HD11	1.97	0.47
2:D:558:ASN:HD21	2:F:562:PHE:C	2.22	0.46
1:E:140:LEU:HD12	1:E:172:VAL:HG23	1.96	0.46
2:B:589:ASP:O	2:B:655:ARG:HB2	2.14	0.46
2:F:184:VAL:HG12	2:F:218:LEU:HD11	1.98	0.46
2:F:478:HIS:NE2	2:F:502:LYS:HG3	2.30	0.46
2:B:326:LEU:O	2:B:327:LYS:HD3	2.15	0.46
2:B:502:LYS:HB3	2:B:502:LYS:HE2	1.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD12	1:C:362:TYR:CE2	2.51	0.46
2:D:35:ALA:HA	2:D:299:LYS:HG2	1.96	0.46
2:D:54:ILE:HB	2:D:71:MET:HB2	1.98	0.46
1:E:279:VAL:HG12	4:E:543:HOH:O	2.15	0.46
2:H:163:SER:HB2	4:H:888:HOH:O	2.16	0.46
1:A:309:CYS:HG	1:A:348:TYR:HE1	1.47	0.46
2:D:590:MET:HB3	2:D:590:MET:HE2	1.66	0.46
2:D:192:LEU:HB2	2:D:206:LEU:HB2	1.98	0.46
2:F:121:LYS:HD2	2:F:137:LEU:HD21	1.98	0.46
2:B:472:GLU:OE2	2:B:508:GLN:HG2	2.15	0.45
2:D:303:ASP:O	2:D:310:PRO:HD2	2.15	0.45
2:D:233:THR:HG21	2:D:249:ARG:HH11	1.82	0.45
2:D:261:ASN:HD21	2:D:265:THR:HG22	1.81	0.45
1:C:286:LEU:O	1:C:287:PHE:HB2	2.16	0.45
2:D:307:ASP:HB3	2:D:308:PRO:HD3	1.95	0.45
2:D:601:TYR:HD1	2:D:639:ILE:HD11	1.82	0.45
2:B:261:ASN:HD21	2:B:265:THR:HG22	1.82	0.45
1:C:284:LEU:HD11	1:C:366:TYR:OH	2.16	0.45
2:H:590:MET:HE3	2:H:590:MET:HB2	1.80	0.45
2:B:192:LEU:HB2	2:B:206:LEU:HB2	1.98	0.45
2:D:381:ASN:O	2:D:400:LYS:HE3	2.16	0.45
2:F:260:VAL:O	2:F:304:ARG:NH2	2.50	0.45
2:H:326:LEU:O	2:H:327:LYS:HD2	2.17	0.45
2:D:153:THR:CG2	2:D:156:ASN:H	2.30	0.45
2:H:39:ASP:HB2	2:H:83:LEU:HD11	1.99	0.45
2:H:459:LYS:N	2:H:459:LYS:CD	2.79	0.45
2:F:261:ASN:HD21	2:F:265:THR:CG2	2.29	0.45
1:A:102:PRO:HA	1:A:103:PRO:HD3	1.87	0.45
1:A:309:CYS:HG	1:A:348:TYR:HD1	1.34	0.45
2:B:459:LYS:HD2	2:B:590:MET:HE1	1.98	0.45
2:B:561:LYS:HG2	2:B:562:PHE:O	2.17	0.45
1:C:140:LEU:HD11	1:C:171:TRP:CZ2	2.52	0.44
2:F:54:ILE:HB	2:F:71:MET:HB2	1.99	0.44
1:C:170:THR:HB	1:C:173:HIS:ND1	2.31	0.44
2:H:510:PRO:HA	2:H:511:PRO:HD3	1.86	0.44
2:D:439:PHE:CE1	2:D:553:ILE:HG13	2.51	0.44
2:F:133:ALA:HB2	2:F:143:LEU:HD23	1.99	0.44
2:B:91:ILE:HD13	2:B:132:VAL:HG21	2.00	0.44
1:E:297:ASP:N	4:E:511:HOH:O	2.49	0.44
2:F:15:VAL:HG22	2:F:547:PRO:HG3	1.98	0.44
2:H:71:MET:HB3	2:H:102:TRP:CZ3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ASN:HD21	2:B:265:THR:CG2	2.30	0.44
2:B:413:MET:HE3	2:B:660:PHE:HB3	2.00	0.44
2:D:30:ARG:NH2	4:D:740:HOH:O	2.51	0.44
1:E:307:VAL:HG23	1:E:319:ILE:HG13	1.98	0.44
2:F:482:MET:HE3	2:F:482:MET:HB2	1.84	0.44
2:H:561:LYS:HE3	2:H:561:LYS:HB3	1.71	0.44
2:H:326:LEU:C	2:H:327:LYS:HD2	2.43	0.43
1:G:246:MET:HE3	1:G:247:LYS:C	2.43	0.43
2:B:373:ARG:HH12	2:B:388:ASP:CG	2.24	0.43
1:C:300:TYR:CE2	1:C:368:SER:HB3	2.53	0.43
2:B:144:TRP:HB3	2:B:149:LEU:HD11	2.00	0.43
2:H:347:THR:CG2	2:H:348:PRO:HD2	2.48	0.43
2:B:194:VAL:HB	2:B:204:MET:HG2	2.01	0.43
1:E:67:PHE:O	1:E:71:VAL:HG13	2.19	0.43
2:H:373:ARG:NH1	2:H:388:ASP:OD1	2.51	0.43
2:B:593:VAL:HG13	2:B:641:LEU:HD12	2.00	0.43
2:D:552:ASP:HB3	4:D:702:HOH:O	2.19	0.43
1:E:186:CYS:O	1:E:190:GLU:HA	2.19	0.43
2:F:561:LYS:HG2	2:F:562:PHE:O	2.19	0.43
1:G:186:CYS:O	1:G:190:GLU:HA	2.18	0.43
2:H:106:LYS:NZ	4:H:722:HOH:O	2.46	0.43
2:H:248:TYR:CE2	2:H:284:PRO:HG3	2.54	0.43
2:H:459:LYS:HG2	2:H:590:MET:HE1	2.00	0.43
1:A:301:ASP:OD2	1:A:369:ARG:HD3	2.19	0.43
1:C:185:ARG:NH1	4:C:509:HOH:O	2.38	0.43
1:C:305:VAL:HG12	1:C:307:VAL:CG2	2.49	0.43
1:E:219:PHE:CE1	1:E:247:LYS:HB2	2.54	0.43
2:B:71:MET:HE3	2:B:107:GLY:HA2	2.01	0.42
1:C:283:GLU:C	1:C:284:LEU:HD12	2.44	0.42
2:B:206:LEU:HB3	2:B:237:TRP:CZ3	2.55	0.42
2:B:282:ARG:H	2:B:282:ARG:HG2	1.54	0.42
2:B:373:ARG:NH2	4:B:724:HOH:O	2.46	0.42
1:C:227:SER:O	1:C:230:LYS:HG3	2.19	0.42
2:B:85:CYS:O	2:B:88:LYS:HE3	2.19	0.42
2:B:535:GLY:HA3	2:B:538:GLU:OE1	2.18	0.42
2:H:88:LYS:HE2	2:H:88:LYS:HB3	1.88	0.42
1:C:143:GLU:HA	1:C:146:GLN:HE21	1.84	0.42
2:D:191:VAL:HG22	2:D:207:LYS:HG2	2.01	0.42
2:D:211:ASP:OD1	2:D:212:ASN:N	2.39	0.42
2:B:464:GLY:O	2:B:468:GLN:HG3	2.19	0.42
1:C:201:ASP:OD1	1:C:201:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:ARG:HA	2:D:57:TRP:O	2.20	0.42
2:D:306:ALA:O	2:D:307:ASP:C	2.62	0.42
1:E:311:SER:OG	1:E:312:GLY:N	2.52	0.42
2:B:568:TYR:CG	2:B:582:LYS:HE3	2.54	0.42
1:G:301:ASP:OD2	1:G:369:ARG:HD3	2.20	0.42
2:B:121:LYS:HE2	4:B:761:HOH:O	2.20	0.42
2:F:629:GLU:HG2	2:F:630:ASP:N	2.35	0.41
2:B:358:LYS:HD2	2:B:359:GLY:H	1.84	0.41
2:F:194:VAL:HB	2:F:204:MET:HG2	2.02	0.41
1:A:67:VAL:HG21	1:A:88:PHE:CD2	2.56	0.41
2:B:307:ASP:CB	2:B:308:PRO:CD	2.96	0.41
2:B:358:LYS:HD2	2:B:358:LYS:HA	1.76	0.41
2:D:27:LYS:NZ	4:D:716:HOH:O	2.54	0.41
2:H:307:ASP:CB	2:H:308:PRO:CD	2.98	0.41
2:B:347:THR:HA	2:B:348:PRO:HD3	1.75	0.41
2:F:261:ASN:HD21	2:F:265:THR:HG23	1.85	0.41
2:F:367:HIS:CD2	2:F:369:LEU:HD13	2.55	0.41
2:H:662:TRP:CZ2	2:H:664:SER:HB2	2.55	0.41
1:C:196:ASP:OD2	1:C:249:LYS:NZ	2.40	0.41
2:D:114:ARG:CZ	4:D:703:HOH:O	2.67	0.41
1:E:68:ARG:O	1:E:72:LEU:HG	2.20	0.41
2:F:527:ARG:NH2	4:F:725:HOH:O	2.40	0.41
2:F:83:LEU:HD22	2:F:87:GLY:HA2	2.03	0.41
2:D:19:TYR:CE1	2:D:466:LEU:HD21	2.56	0.41
2:D:527:ARG:HD3	2:D:528:LEU:N	2.36	0.41
1:C:63:PHE:O	1:C:67:VAL:HG13	2.20	0.41
2:D:662:TRP:CZ2	2:D:664:SER:HB2	2.56	0.41
2:F:283:ASN:HA	2:F:284:PRO:HD2	1.84	0.41
1:G:142:GLU:HA	1:G:145:LYS:HB3	2.02	0.41
2:H:82:VAL:HG11	2:H:125:TYR:HB2	2.03	0.41
2:B:481:PRO:HB3	2:H:564:LYS:NZ	2.35	0.41
2:F:510:PRO:HA	2:F:511:PRO:HD3	1.87	0.41
2:B:584:ARG:HD3	4:B:864:HOH:O	2.21	0.40
1:A:323:LYS:NZ	1:A:325:HIS:O	2.37	0.40
2:F:640:GLU:HG3	2:F:675:LYS:HD3	2.04	0.40
2:F:649:ASP:HA	2:F:650:PRO:HD2	1.89	0.40
2:B:654:LEU:HD23	2:B:654:LEU:HA	1.91	0.40
2:H:39:ASP:OD1	4:H:701:HOH:O	2.22	0.40
2:H:265:THR:OG1	2:H:282:ARG:HD2	2.21	0.40
1:C:79:SER:OG	1:C:80:LEU:N	2.55	0.40
2:F:287:ARG:HE	2:F:287:ARG:HB3	1.72	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:O	1:A:67:VAL:HG22	2.20	0.40
2:B:572:HIS:CD2	2:B:642:LEU:HD22	2.57	0.40
2:F:593:VAL:HG12	2:F:650:PRO:HA	2.02	0.40
2:H:184:VAL:HG12	2:H:218:LEU:HD11	2.03	0.40
2:H:347:THR:HG23	2:H:348:PRO:HD2	2.04	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)
2:D:249:ARG:NH2	1:E:338:LYS:O[2_555]	2.11	0.09

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	221/331 (67%)	211 (96%)	10 (4%)	0	100	100
1	C	218/331 (66%)	212 (97%)	6 (3%)	0	100	100
1	E	204/331 (62%)	197 (97%)	7 (3%)	0	100	100
1	G	205/331 (62%)	198 (97%)	6 (3%)	1 (0%)	24	31
2	B	583/677 (86%)	558 (96%)	23 (4%)	2 (0%)	36	46
2	D	587/677 (87%)	570 (97%)	17 (3%)	0	100	100
2	F	590/677 (87%)	570 (97%)	19 (3%)	1 (0%)	43	55
2	H	584/677 (86%)	563 (96%)	20 (3%)	1 (0%)	43	55
All	All	3192/4032 (79%)	3079 (96%)	108 (3%)	5 (0%)	43	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	334	ASP
2	B	73	HIS
2	F	73	HIS
2	B	307	ASP
2	H	307	ASP

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	202/305 (66%)	193 (96%)	9 (4%)	24	37
1	C	207/305 (68%)	201 (97%)	6 (3%)	37	55
1	E	186/305 (61%)	182 (98%)	4 (2%)	45	65
1	G	188/305 (62%)	185 (98%)	3 (2%)	55	73
2	B	518/597 (87%)	507 (98%)	11 (2%)	47	66
2	D	519/597 (87%)	505 (97%)	14 (3%)	39	58
2	F	525/597 (88%)	513 (98%)	12 (2%)	44	63
2	H	514/597 (86%)	497 (97%)	17 (3%)	33	50
All	All	2859/3608 (79%)	2783 (97%)	76 (3%)	39	58

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	66	LYS
1	A	175	ILE
1	A	202	LEU
1	A	234	GLU
1	A	279	VAL
1	A	284	LEU
1	A	323	LYS
1	A	360	SER
2	B	27	LYS
2	B	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	73	HIS
2	B	75	THR
2	B	127	LYS
2	B	198	ARG
2	B	250	VAL
2	B	369	LEU
2	B	467	LEU
2	B	502	LYS
2	B	675	LYS
1	C	42	VAL
1	C	105	LYS
1	C	172	VAL
1	C	250	LYS
1	C	279	VAL
1	C	359	GLU
2	D	24	GLU
2	D	30	ARG
2	D	73	HIS
2	D	82	VAL
2	D	198	ARG
2	D	372	LYS
2	D	429	LEU
2	D	527	ARG
2	D	546	VAL
2	D	561	LYS
2	D	581	LYS
2	D	593	VAL
2	D	594	ARG
2	D	605	ILE
1	E	69	GLU
1	E	244	LYS
1	E	306	VAL
1	E	369	ARG
2	F	15	VAL
2	F	25	VAL
2	F	30	ARG
2	F	73	HIS
2	F	129	LYS
2	F	198	ARG
2	F	282	ARG
2	F	369	LEU
2	F	390	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	509	VAL
2	F	593	VAL
2	F	631	ILE
1	G	80	LEU
1	G	204	VAL
1	G	246	MET
2	H	14	LYS
2	H	73	HIS
2	H	84	CYS
2	H	198	ARG
2	H	282	ARG
2	H	307	ASP
2	H	365	GLN
2	H	380	THR
2	H	436	SER
2	H	443	VAL
2	H	500	VAL
2	H	502	LYS
2	H	509	VAL
2	H	527	ARG
2	H	540	MET
2	H	604	ILE
2	H	644	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS
2	B	224	GLN
2	B	508	GLN
2	B	548	GLN
2	B	659	HIS
1	C	146	GLN
2	D	16	GLN
2	D	43	ASN
2	D	224	GLN
2	D	283	ASN
2	D	382	ASN
2	F	16	GLN
2	F	322	ASN
2	F	365	GLN
1	G	89	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	239/331 (72%)	0.47	21 (8%) 15 17	25, 49, 80, 92	0
1	C	236/331 (71%)	0.63	26 (11%) 10 11	27, 53, 84, 95	0
1	E	222/331 (67%)	0.68	27 (12%) 8 9	25, 54, 84, 89	0
1	G	224/331 (67%)	0.73	23 (10%) 12 13	24, 55, 87, 97	1 (0%)
2	B	595/677 (87%)	-0.13	15 (2%) 58 60	23, 35, 57, 90	0
2	D	597/677 (88%)	-0.19	15 (2%) 58 60	21, 33, 60, 81	0
2	F	600/677 (88%)	-0.24	9 (1%) 72 73	22, 31, 58, 73	0
2	H	594/677 (87%)	-0.09	14 (2%) 59 62	20, 32, 70, 87	0
All	All	3307/4032 (82%)	0.06	150 (4%) 38 40	20, 37, 73, 97	1 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	VAL	5.3
1	C	287	PHE	5.1
2	H	573	ALA	4.6
2	H	500	VAL	4.5
1	A	279	VAL	4.4
1	C	340	ASP	4.2
1	E	344	ILE	4.0
1	G	344	ILE	4.0
2	B	158	THR	4.0
2	F	328	GLY	3.9
2	D	328	GLY	3.9
2	B	307	ASP	3.8
1	E	287	PHE	3.8
1	E	206	VAL	3.8
1	A	297	ASP	3.8
1	C	344	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	333	ASP	3.7
1	C	343	ALA	3.6
1	A	287	PHE	3.6
1	G	279	VAL	3.6
2	D	500	VAL	3.6
1	C	280	PHE	3.6
2	B	607	LEU	3.6
1	C	65	GLU	3.5
1	A	102	PRO	3.4
1	G	44	PHE	3.4
1	G	125	ALA	3.4
1	E	169	PRO	3.3
1	G	313	PRO	3.3
1	C	279	VAL	3.3
1	G	80	LEU	3.3
1	E	313	PRO	3.3
2	H	673	ARG	3.2
1	G	339	ILE	3.2
2	D	307	ASP	3.2
2	H	307	ASP	3.2
1	A	309	CYS	3.2
2	D	72	GLU	3.2
2	B	328	GLY	3.1
2	F	307	ASP	3.1
1	E	102	PRO	3.1
1	G	41	LEU	3.1
2	D	159	VAL	3.0
2	F	287	ARG	3.0
2	H	581	LYS	3.0
2	H	604	ILE	3.0
1	C	210	THR	3.0
1	E	319	ILE	2.9
1	G	331	PHE	2.9
2	D	62	HIS	2.9
2	D	605	ILE	2.9
2	D	631	ILE	2.9
2	H	62	HIS	2.9
1	A	335	ILE	2.9
2	B	155	SER	2.8
1	E	106	PHE	2.8
1	E	345	GLU	2.8
1	G	359	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	319	ILE	2.8
1	E	347	PHE	2.8
1	A	336	VAL	2.8
1	C	339	ILE	2.8
1	G	146	GLN	2.8
1	G	87	LEU	2.8
1	E	103	PRO	2.7
1	C	284	LEU	2.7
2	F	522	GLY	2.7
2	D	308	PRO	2.7
2	F	573	ALA	2.7
1	A	42	VAL	2.7
1	E	342	GLN	2.7
1	G	347	PHE	2.7
1	A	348	TYR	2.6
1	C	70	TYR	2.6
1	E	310	GLY	2.6
1	C	342	GLN	2.6
1	E	48	PHE	2.6
1	G	335	ILE	2.6
1	G	287	PHE	2.6
1	E	348	TYR	2.6
1	A	327	PHE	2.5
2	B	153	THR	2.5
1	C	335	ILE	2.5
1	G	205	ASP	2.5
1	A	169	PRO	2.5
2	D	522	GLY	2.5
1	E	139	ILE	2.5
1	E	334	ASP	2.5
1	C	169	PRO	2.5
1	C	125	ALA	2.4
1	E	143	GLU	2.4
1	C	327	PHE	2.4
2	B	500	VAL	2.4
2	H	328	GLY	2.4
1	A	345	GLU	2.4
1	A	313	PRO	2.4
2	B	286	ILE	2.4
1	E	72	LEU	2.4
2	B	156	ASN	2.3
2	D	675	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	306	VAL	2.3
1	C	336	VAL	2.3
1	C	146	GLN	2.3
2	F	580	LEU	2.3
2	D	60	ASN	2.3
2	H	665	GLY	2.3
1	E	73	ALA	2.3
2	H	285	ASP	2.3
1	C	229	TYR	2.3
1	C	328	TRP	2.3
2	B	154	ALA	2.3
2	B	573	ALA	2.3
2	D	573	ALA	2.3
1	E	325	HIS	2.3
1	G	358	SER	2.3
1	A	357	ASN	2.2
2	H	630	ASP	2.2
1	A	341	ALA	2.2
1	G	70	TYR	2.2
1	E	95	ILE	2.2
2	B	191	VAL	2.2
1	A	342	GLN	2.2
1	A	41	LEU	2.2
2	D	645	ASP	2.2
2	F	665	GLY	2.2
1	C	144	ARG	2.2
2	D	581	LYS	2.2
1	C	341	ALA	2.2
1	C	329	LEU	2.1
1	E	105	LYS	2.1
1	G	210	THR	2.1
1	E	141	GLN	2.1
1	E	253	MET	2.1
1	G	68	LEU	2.1
1	A	347	PHE	2.1
1	G	85	ALA	2.1
1	G	147	GLU	2.1
2	B	501	GLN	2.1
2	H	631	ILE	2.1
2	F	308	PRO	2.1
1	C	111	ARG	2.1
2	B	540	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	49	GLY	2.0
1	A	210	THR	2.0
2	B	629	GLU	2.0
2	H	158	THR	2.0
1	E	91	LEU	2.0
2	F	285	ASP	2.0
1	A	344	ILE	2.0
2	H	286	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($\text{\AA}^2$)	Q<0.9
3	ZN	G	401	1/1	0.97	0.12	45,45,45,45	0
3	ZN	C	401	1/1	0.99	0.02	30,30,30,30	0
3	ZN	E	401	1/1	1.00	0.04	32,32,32,32	0
3	ZN	A	401	1/1	1.00	0.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.