



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 06:19 PM JST

PDB ID : 7W3U
Title : USP34 catalytic domain in complex with UbPA
Authors : Xu, G.L.; Ming, Z.H.
Deposited on : 2021-11-26
Resolution : 3.13 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
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) : 2.28.1

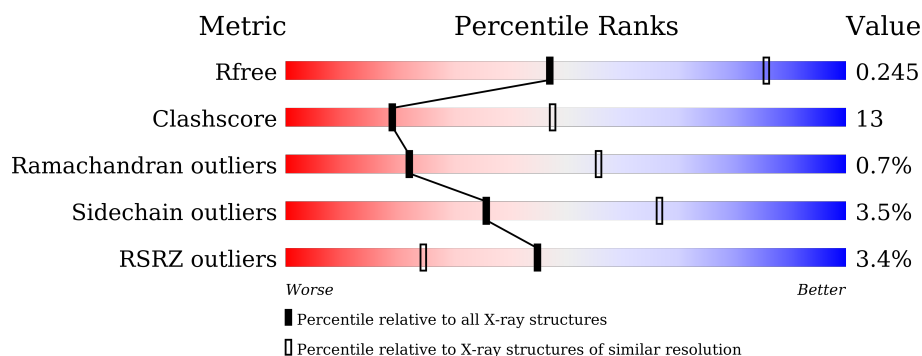
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	384	<div> <div>2%</div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	B	384	<div> <div>3%</div> <div>63%</div> <div>23%</div> <div>•</div> <div>12%</div> </div>
1	C	384	<div> <div>6%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>13%</div> </div>
2	D	75	<div> <div>64%</div> <div>36%</div> </div>
2	E	75	<div> <div>63%</div> <div>36%</div> <div>•</div> </div>
2	F	75	<div> <div>65%</div> <div>31%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AYE	A	2302	-	-	X	-
4	AYE	E	101	-	-	X	-
4	AYE	F	101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10120 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 34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2815	1799	450	538	28			
1	B	338	Total	C	N	O	S	0	0	0
			2768	1766	444	531	27			
1	C	333	Total	C	N	O	S	0	0	0
			2731	1746	439	519	27			

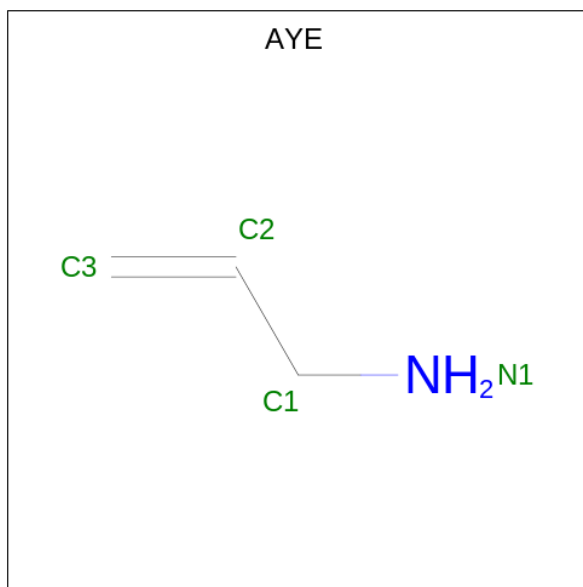
- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	E	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			
2	F	75	Total	C	N	O	S	0	0	0
			597	376	104	116	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

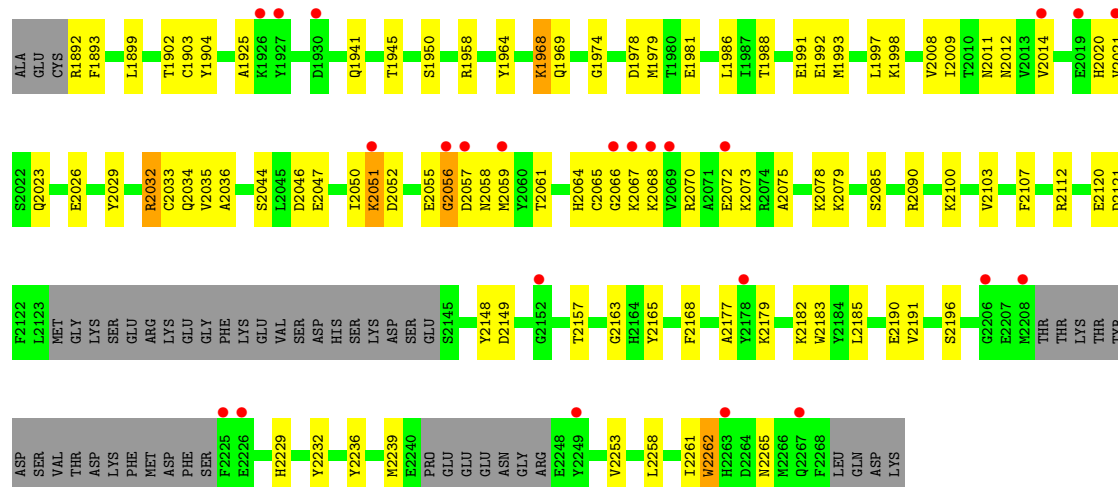
- Molecule 4 is prop-2-en-1-amine (three-letter code: AYE) (formula: C₃H₇N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			4	3	1		
4	E	1	Total	C	N	0	0
			4	3	1		
4	F	1	Total	C	N	0	0
			4	3	1		

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 34





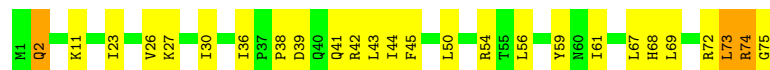
● Molecule 2: Polyubiquitin-B



● Molecule 2: Polyubiquitin-B



● Molecule 2: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	192.02Å 71.33Å 111.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.60 – 3.13 23.67 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.60-3.13) 89.5 (23.67-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.10Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.217 , 0.245 0.216 , 0.245	Depositor DCC
R_{free} test set	1988 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10120	wwPDB-VP
Average B, all atoms (Å ²)	97.0	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.*

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, AYE

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	0.30	0/2880	0.48	0/3881
1	B	0.28	0/2831	0.48	1/3816 (0.0%)
1	C	0.27	0/2794	0.47	0/3765
2	D	0.26	0/603	0.52	0/811
2	E	0.28	0/603	0.52	0/811
2	F	0.26	0/603	0.49	0/811
All	All	0.28	0/10314	0.48	1/13895 (0.0%)

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
2	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2084	LEU	CA-CB-CG	5.58	128.14	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	58	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2815	0	2712	72	0
1	B	2768	0	2665	68	1
1	C	2731	0	2636	65	1
2	D	597	0	626	36	0
2	E	597	0	626	32	0
2	F	597	0	626	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	6	17	0
4	E	4	0	4	5	0
4	F	4	0	6	4	0
All	All	10120	0	9907	261	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 13.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2302:AYE:C1	2:D:75:GLY:O	1.82	1.26
4:A:2302:AYE:H1	2:D:75:GLY:O	1.07	1.24
1:C:1903:CYS:H	4:F:101:AYE:H3A	1.01	1.14
4:A:2302:AYE:H1	2:D:75:GLY:C	1.71	1.10
2:E:2:GLN:OE1	2:E:14:THR:HG21	1.59	1.03
2:E:2:GLN:HG3	2:E:14:THR:HG23	1.40	1.02
1:C:1903:CYS:N	4:F:101:AYE:H3A	1.60	1.02
1:A:1903:CYS:HB2	4:A:2302:AYE:HN1	1.31	0.95
1:B:1903:CYS:H	4:E:101:AYE:H3A	1.35	0.90
1:C:1903:CYS:H	4:F:101:AYE:C3	1.87	0.86
2:E:2:GLN:OE1	2:E:14:THR:CG2	2.28	0.81
2:F:56:LEU:HG	2:F:61:ILE:HD11	1.62	0.80
1:C:1950:SER:HB2	1:C:2261:ILE:HD11	1.64	0.78
2:E:2:GLN:CG	2:E:14:THR:HG23	2.13	0.78
2:E:2:GLN:HG3	2:E:14:THR:CG2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ARG:HH11	2:E:55:THR:H	1.30	0.76
1:C:2112:ARG:NH1	1:C:2239:MET:SD	2.59	0.75
1:A:2058:ASN:HD22	2:D:14:THR:H	1.36	0.73
1:A:1903:CYS:CB	4:A:2302:AYE:HN1	2.02	0.72
1:C:1893:PHE:HB2	1:C:2191:VAL:HG11	1.72	0.72
1:B:2253:VAL:HG13	1:B:2258:LEU:HD11	1.70	0.72
1:C:2008:VAL:HG12	1:C:2079:LYS:HG2	1.73	0.71
1:C:2014:VAL:HG12	1:C:2021:VAL:HG22	1.73	0.71
2:D:43:LEU:HD23	2:D:67:LEU:HD23	1.72	0.70
1:B:2154:THR:HB	1:B:2233:MET:HB3	1.73	0.70
1:A:2248:GLU:N	1:A:2248:GLU:OE1	2.26	0.69
1:C:2034:GLN:O	1:C:2044:SER:OG	2.09	0.69
1:C:2163:GLY:O	4:F:101:AYE:N1	2.24	0.68
1:A:2176:HIS:HA	1:A:2179:LYS:HE3	1.76	0.68
1:B:2112:ARG:NH2	1:B:2147:GLU:OE1	2.27	0.67
1:A:2100:LYS:NZ	2:D:72:ARG:O	2.26	0.67
1:A:2145:SER:O	1:A:2238:ARG:NH1	2.25	0.67
1:A:2156:HIS:CG	2:D:73:LEU:HD11	2.29	0.67
1:A:2165:TYR:HD2	4:A:2302:AYE:N1	1.93	0.67
1:B:2032:ARG:HG3	1:B:2032:ARG:HH11	1.61	0.65
1:B:1916:PRO:HG3	1:B:2173:VAL:HG22	1.78	0.65
2:D:56:LEU:HG	2:D:61:ILE:HD11	1.78	0.65
1:A:2058:ASN:ND2	2:D:14:THR:H	1.93	0.65
1:B:1928:SER:HB2	1:B:1931:MET:HB3	1.79	0.64
1:B:2054:LEU:O	1:B:2058:ASN:ND2	2.30	0.64
1:A:2055:GLU:OE1	1:A:2070:ARG:NH1	2.31	0.63
1:B:1892:ARG:HG3	1:B:1893:PHE:H	1.64	0.63
1:B:2148:TYR:HB3	1:B:2236:TYR:HB3	1.80	0.62
1:C:2065:CYS:O	1:C:2067:LYS:N	2.33	0.62
4:A:2302:AYE:N1	2:D:75:GLY:O	2.32	0.62
1:A:2210:THR:HA	1:B:2179:LYS:NZ	2.15	0.61
2:D:5:VAL:HB	2:D:13:ILE:HG12	1.81	0.61
1:A:2058:ASN:ND2	2:D:13:ILE:HA	2.16	0.61
1:A:2164:HIS:HA	4:A:2302:AYE:H1A	1.82	0.61
1:A:2120:GLU:HG3	1:A:2124:MET:HG3	1.83	0.61
1:B:2061:THR:H	2:E:2:GLN:HE22	1.49	0.61
1:B:2084:LEU:HD12	1:B:2236:TYR:HB2	1.82	0.61
2:E:42:ARG:HB2	2:E:70:VAL:HG23	1.83	0.60
1:A:2058:ASN:HD22	2:D:14:THR:N	1.97	0.60
1:B:1903:CYS:H	4:E:101:AYE:C3	2.12	0.59
1:C:2165:TYR:CE2	2:F:75:GLY:HA3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2017:ASP:HB2	1:B:2069:VAL:HG13	1.86	0.58
1:A:2014:VAL:HG23	1:A:2072:GLU:HG3	1.86	0.57
2:F:45:PHE:CE2	2:F:61:ILE:HG22	2.39	0.57
1:C:2011:ASN:HB3	1:C:2075:ALA:HA	1.85	0.57
1:A:2112:ARG:NH1	1:A:2147:GLU:OE1	2.38	0.56
1:C:1991:GLU:OE1	1:C:2029:TYR:OH	2.20	0.56
1:B:2009:ILE:HD11	1:B:2075:ALA:HB1	1.87	0.56
2:E:54:ARG:NH1	2:E:55:THR:OG1	2.38	0.56
2:F:39:ASP:OD1	2:F:39:ASP:N	2.39	0.56
1:A:2156:HIS:CG	2:D:73:LEU:CD1	2.88	0.56
2:D:39:ASP:OD1	2:D:39:ASP:N	2.34	0.56
1:C:2014:VAL:HG23	1:C:2072:GLU:HG2	1.88	0.56
1:A:1929:GLU:OE2	1:A:1934:LYS:NZ	2.39	0.56
1:C:2008:VAL:HG13	1:C:2078:LYS:HB3	1.87	0.56
2:F:41:GLN:HB3	2:F:69:LEU:HD11	1.86	0.56
1:A:2144:GLU:OE1	1:A:2144:GLU:N	2.38	0.56
1:A:2154:THR:HB	1:A:2233:MET:HB3	1.88	0.55
1:B:2151:ILE:HD13	1:B:2237:LYS:HB2	1.86	0.55
1:C:2057:ASP:OD1	1:C:2058:ASN:N	2.38	0.55
1:C:2157:THR:HB	1:C:2229:HIS:HB3	1.87	0.55
1:A:1928:SER:HB2	1:A:1931:MET:HB3	1.87	0.55
2:E:3:ILE:HD13	2:E:17:VAL:HG21	1.89	0.55
1:B:2015:SER:OG	1:B:2069:VAL:HG12	2.07	0.55
2:D:17:VAL:HG12	2:D:29:LYS:HE2	1.89	0.55
1:B:2164:HIS:HA	4:E:101:AYE:H1A	1.88	0.55
1:A:2060:TYR:O	2:D:2:GLN:NE2	2.40	0.55
1:C:2032:ARG:HH21	2:F:44:ILE:HD13	1.71	0.55
1:A:1937:LEU:HB2	1:A:1993:MET:SD	2.47	0.54
1:A:2059:MET:HB3	1:A:2068:LYS:HB3	1.88	0.54
2:E:24:GLU:N	2:E:24:GLU:OE1	2.40	0.54
1:C:2112:ARG:NH1	1:C:2149:ASP:OD1	2.36	0.54
1:A:2019:GLU:OE1	1:A:2019:GLU:N	2.40	0.54
2:E:54:ARG:HH22	2:E:58:ASP:HB2	1.73	0.54
1:A:2156:HIS:CD2	2:D:73:LEU:CD1	2.91	0.54
2:F:50:LEU:HA	2:F:59:TYR:CZ	2.43	0.53
1:C:1991:GLU:HG3	1:C:1998:LYS:HG3	1.90	0.53
1:B:2046:ASP:O	1:B:2050:ILE:HB	2.09	0.53
1:A:2049:THR:HG21	1:A:2118:TYR:HB3	1.89	0.53
1:A:1903:CYS:CB	4:A:2302:AYE:N1	2.71	0.53
1:C:2012:ASN:HB3	1:C:2023:GLN:HB2	1.89	0.53
1:A:1901:ALA:O	4:A:2302:AYE:H3A	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2102:LYS:HE2	1:A:2158:GLY:O	2.09	0.52
1:C:1925:ALA:HB3	1:C:1941:GLN:HE21	1.74	0.52
1:C:2052:ASP:HB3	1:C:2072:GLU:HB2	1.91	0.52
1:A:1903:CYS:HB2	4:A:2302:AYE:N1	2.13	0.52
1:B:2159:THR:HG22	1:B:2160:ALA:H	1.73	0.52
2:D:63:LYS:HG2	2:D:64:GLU:HG3	1.91	0.52
2:E:54:ARG:NH2	2:E:58:ASP:HB2	2.24	0.52
1:C:2047:GLU:OE2	2:F:11:LYS:HE3	2.10	0.52
1:C:2177:ALA:HB1	1:C:2182:LYS:HB2	1.91	0.52
1:A:2165:TYR:CD2	4:A:2302:AYE:N1	2.76	0.51
1:A:2058:ASN:HD21	2:D:13:ILE:HB	1.76	0.51
1:C:2052:ASP:HA	1:C:2073:LYS:O	2.09	0.51
1:C:2036:ALA:HB2	1:C:2103:VAL:HG21	1.93	0.51
1:B:2024:THR:HG22	1:B:2025:ALA:H	1.75	0.51
2:D:55:THR:HG22	2:D:57:SER:H	1.76	0.50
1:A:1892:ARG:CZ	1:A:1892:ARG:HB2	2.42	0.50
1:C:2061:THR:HB	2:F:2:GLN:HG2	1.93	0.50
1:C:1964:TYR:HE2	1:C:1986:LEU:HD13	1.76	0.50
1:B:2060:TYR:OH	2:E:64:GLU:OE2	2.29	0.50
2:E:75:GLY:O	4:E:101:AYE:H3	2.12	0.50
1:C:1945:THR:HG23	1:C:2253:VAL:HG11	1.94	0.50
1:C:1978:ASP:HB2	2:F:72:ARG:HB3	1.93	0.50
1:C:2055:GLU:HG2	1:C:2056:GLY:N	2.26	0.50
1:B:1903:CYS:N	4:E:101:AYE:H3A	2.16	0.49
1:A:1990:ILE:HA	1:A:1993:MET:HG3	1.95	0.49
2:E:44:ILE:HB	2:E:68:HIS:HB2	1.94	0.49
1:A:1904:TYR:CZ	1:A:1977:LYS:HD3	2.47	0.49
1:A:1990:ILE:HA	1:A:1993:MET:HE2	1.94	0.49
2:D:27:LYS:HB3	2:D:38:PRO:HB3	1.94	0.49
1:C:1925:ALA:HB3	1:C:1941:GLN:NE2	2.28	0.49
2:F:27:LYS:HB3	2:F:38:PRO:HB3	1.95	0.49
1:B:1904:TYR:CZ	1:B:1977:LYS:HB2	2.47	0.49
1:A:2187:ASN:O	1:A:2187:ASN:ND2	2.41	0.48
4:A:2302:AYE:C3	2:D:75:GLY:O	2.61	0.48
2:D:19:PRO:HA	2:D:56:LEU:HD22	1.95	0.48
1:C:2050:ILE:HG23	1:C:2051:LYS:HB2	1.95	0.48
1:A:2156:HIS:ND1	2:D:73:LEU:HD11	2.28	0.48
1:C:2012:ASN:OD1	1:C:2012:ASN:N	2.44	0.48
1:A:1892:ARG:HB2	1:A:1892:ARG:NH1	2.28	0.48
1:A:2009:ILE:HG13	1:A:2028:PHE:CD2	2.49	0.48
1:B:1976:GLN:HB3	2:E:75:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:PHE:HB2	2:F:67:LEU:HD12	1.96	0.47
1:B:2156:HIS:HB2	1:B:2165:TYR:CE1	2.49	0.47
1:A:2039:LYS:HB3	1:A:2039:LYS:HE3	1.77	0.47
4:A:2302:AYE:C2	2:D:75:GLY:O	2.58	0.47
1:B:2091:TYR:CE1	2:E:71:LEU:HB2	2.50	0.47
4:A:2302:AYE:H3	2:D:75:GLY:O	2.14	0.47
1:C:1968:LYS:HD3	1:C:1969:GLN:HG3	1.96	0.47
2:F:36:ILE:O	2:F:41:GLN:NE2	2.46	0.47
1:A:1920:GLN:HE22	1:A:2252:ASP:H	1.61	0.47
2:E:54:ARG:HA	2:E:54:ARG:HD2	1.60	0.47
2:F:73:LEU:HD23	2:F:73:LEU:HA	1.73	0.47
1:A:1920:GLN:OE1	1:A:2251:PHE:HA	2.15	0.47
1:A:2195:ASP:OD2	1:B:2196:SER:OG	2.31	0.47
1:B:2121:ASP:O	1:B:2123:LEU:N	2.47	0.47
1:B:1904:TYR:O	1:B:1908:THR:OG1	2.25	0.47
1:C:2020:HIS:CE1	1:C:2064:HIS:HB2	2.50	0.47
2:D:45:PHE:CE2	2:D:61:ILE:HG22	2.50	0.47
1:B:2030:THR:HG22	1:B:2085:SER:OG	2.15	0.47
1:C:1904:TYR:HB2	1:C:1979:MET:HA	1.98	0.46
1:B:1904:TYR:CE2	1:B:1977:LYS:HB2	2.50	0.46
1:C:2232:TYR:CD1	2:F:73:LEU:HD12	2.50	0.46
1:A:2035:VAL:HG11	1:A:2090:ARG:HG2	1.97	0.46
1:B:1946:TYR:CD1	1:B:1955:TYR:HB2	2.51	0.46
1:B:1990:ILE:HG23	1:B:1997:LEU:HD13	1.98	0.46
1:B:2008:VAL:HB	1:B:2079:LYS:HB2	1.98	0.46
1:A:2060:TYR:O	1:A:2061:THR:OG1	2.30	0.46
1:C:2090:ARG:NH2	1:C:2107:PHE:HB3	2.31	0.46
1:B:1996:GLU:H	1:B:1996:GLU:CD	2.19	0.46
1:B:1905:LEU:HA	1:B:1982:PHE:CE2	2.51	0.45
1:C:1993:MET:HB2	1:C:1997:LEU:HD12	1.97	0.45
1:A:2061:THR:CG2	1:A:2068:LYS:HE3	2.46	0.45
1:B:2012:ASN:OD1	1:B:2023:GLN:NE2	2.50	0.45
2:E:2:GLN:CD	2:E:14:THR:CG2	2.85	0.45
1:C:2258:LEU:O	1:C:2262:TRP:HB2	2.17	0.45
2:E:61:ILE:HD13	2:E:67:LEU:HD11	1.98	0.45
1:B:2240:GLU:N	1:B:2240:GLU:OE1	2.50	0.45
1:A:1912:LEU:HD21	1:A:1987:ILE:HD11	1.99	0.45
1:A:2204:PHE:HE2	1:B:2112:ARG:CZ	2.29	0.45
1:A:2212:THR:O	1:A:2213:TYR:HB2	2.17	0.45
1:B:2084:LEU:HG	1:B:2148:TYR:CE2	2.52	0.44
1:A:2157:THR:HG23	1:A:2157:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2152:GLY:HA2	1:B:2169:ILE:HA	2.00	0.44
1:B:2225:PHE:CE2	1:C:1958:ARG:HD2	2.53	0.44
2:D:26:VAL:HG21	2:D:56:LEU:HD12	1.99	0.44
1:A:1946:TYR:CD1	1:A:1955:TYR:HB2	2.53	0.44
1:A:2148:TYR:HB3	1:A:2236:TYR:HB3	1.98	0.44
1:B:1958:ARG:O	1:B:1962:LYS:HG3	2.17	0.44
1:B:2054:LEU:HD11	1:B:2071:ALA:HB3	1.99	0.44
2:D:7:THR:HG21	2:D:34:GLU:HG3	1.98	0.44
2:E:37:PRO:HG2	2:E:40:GLN:HB2	1.99	0.44
1:A:1914:MET:HG3	1:A:2169:ILE:HG21	1.98	0.44
2:E:36:ILE:HD12	2:E:69:LEU:HD21	1.98	0.44
2:F:42:ARG:NH2	2:F:44:ILE:HD11	2.33	0.44
1:C:2183:TRP:CD1	1:C:2196:SER:HB3	2.53	0.44
1:B:2058:ASN:HB2	2:E:14:THR:H	1.83	0.44
1:C:2121:ASP:OD1	1:C:2121:ASP:N	2.50	0.44
1:C:2078:LYS:HE2	1:C:2120:GLU:OE2	2.18	0.44
2:D:54:ARG:HA	2:D:54:ARG:HD3	1.60	0.43
2:D:61:ILE:HD12	2:D:67:LEU:HD11	1.98	0.43
2:E:2:GLN:CD	2:E:14:THR:HG23	2.37	0.43
1:A:1897:THR:HB	1:A:1956:ASN:HA	1.99	0.43
1:B:2267:GLN:OE1	1:B:2267:GLN:N	2.52	0.43
2:F:43:LEU:HA	2:F:68:HIS:O	2.19	0.43
1:B:1904:TYR:HB2	1:B:1979:MET:HA	2.00	0.43
1:B:2009:ILE:HG13	1:B:2076:CYS:O	2.18	0.43
1:A:2197:ALA:HB2	1:B:2111:LEU:HD13	2.00	0.43
1:A:2199:LEU:HD23	1:A:2199:LEU:HA	1.87	0.43
1:B:2036:ALA:HB2	1:B:2103:VAL:HG21	2.00	0.43
2:F:26:VAL:O	2:F:30:ILE:N	2.51	0.43
1:A:2179:LYS:HG3	1:B:2106:HIS:CE1	2.53	0.43
1:B:2153:VAL:HG11	1:B:2203:CYS:SG	2.59	0.43
1:C:2100:LYS:HB2	1:C:2100:LYS:HE2	1.75	0.43
1:A:2267:GLN:N	1:A:2267:GLN:OE1	2.52	0.43
2:E:56:LEU:HD22	2:E:61:ILE:HD12	2.01	0.43
1:C:1988:THR:O	1:C:1992:GLU:HG3	2.19	0.42
1:B:2084:LEU:CD1	1:B:2236:TYR:HB2	2.49	0.42
1:B:2159:THR:OG1	1:C:1974:GLY:N	2.52	0.42
2:F:26:VAL:HG21	2:F:56:LEU:HD12	2.01	0.42
2:E:26:VAL:O	2:E:30:ILE:HG13	2.20	0.42
1:B:2108:SER:HA	1:B:2204:PHE:CD1	2.54	0.42
1:C:2168:PHE:CE1	1:C:2185:LEU:HD13	2.54	0.42
2:E:23:ILE:HG12	2:E:54:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1903:CYS:H	4:A:2302:AYE:H3A	1.84	0.42
1:A:2187:ASN:ND2	1:A:2187:ASN:C	2.73	0.42
2:D:45:PHE:HB3	2:D:50:LEU:HD21	2.02	0.42
1:C:1981:GLU:OE2	2:F:72:ARG:NE	2.49	0.42
1:C:2232:TYR:CE1	2:F:73:LEU:HB2	2.55	0.42
1:A:1928:SER:O	1:A:1934:LYS:HD2	2.20	0.42
2:D:2:GLN:HG3	2:D:2:GLN:O	2.20	0.42
1:C:2148:TYR:HB3	1:C:2236:TYR:HB3	2.01	0.42
1:A:2108:SER:OG	1:B:2147:GLU:OE2	2.37	0.41
1:C:1978:ASP:OD2	2:F:72:ARG:HA	2.20	0.41
2:E:37:PRO:HA	2:E:38:PRO:HD3	1.97	0.41
2:F:45:PHE:CZ	2:F:61:ILE:HG22	2.56	0.41
1:B:2166:TYR:HD2	1:B:2185:LEU:HD11	1.86	0.41
2:E:44:ILE:HD13	2:E:49:GLN:HB2	2.02	0.41
1:C:2232:TYR:CZ	2:F:73:LEU:HB2	2.56	0.41
1:B:2009:ILE:HG22	1:B:2028:PHE:HD2	1.86	0.41
1:C:2033:CYS:HB3	1:C:2044:SER:HB3	2.03	0.41
1:C:2035:VAL:HG11	1:C:2090:ARG:HG2	2.02	0.41
1:A:2058:ASN:ND2	2:D:13:ILE:CA	2.81	0.41
1:C:1997:LEU:HD23	1:C:1997:LEU:HA	1.92	0.41
1:B:2051:LYS:HE3	1:B:2051:LYS:HB3	1.87	0.41
2:E:2:GLN:CG	2:E:14:THR:CG2	2.87	0.41
1:A:2062:CYS:HB3	1:A:2065:CYS:HB2	2.02	0.41
1:B:1923:PHE:HD1	1:B:1923:PHE:HA	1.78	0.41
1:B:2167:SER:HB3	1:B:2169:ILE:HG23	2.03	0.41
1:B:2199:LEU:HD23	1:B:2199:LEU:HA	1.94	0.41
1:C:2029:TYR:O	1:C:2085:SER:OG	2.39	0.41
1:C:2179:LYS:HA	1:C:2179:LYS:HD2	1.92	0.41
2:E:23:ILE:HD12	2:E:50:LEU:HD13	2.03	0.41
2:F:23:ILE:HD12	2:F:50:LEU:HD13	2.03	0.41
1:B:2032:ARG:HD3	1:B:2087:ASN:HB3	2.02	0.40
1:B:2104:ASN:HB2	1:B:2226:GLU:HG3	2.02	0.40
1:B:2190:GLU:HG3	1:C:2190:GLU:HG3	2.02	0.40
1:A:2045:LEU:HD21	1:A:2086:PHE:CE1	2.55	0.40
1:B:2210:THR:HG22	1:B:2225:PHE:HE1	1.86	0.40
1:C:1899:LEU:HB2	1:C:1902:THR:HG21	2.02	0.40
1:C:2051:LYS:HA	1:C:2051:LYS:HD2	1.77	0.40
1:A:2061:THR:H	1:A:2068:LYS:HA	1.86	0.40
1:A:2163:GLY:O	4:A:2302:AYE:H1A	2.21	0.40
1:C:2009:ILE:N	1:C:2026:GLU:O	2.47	0.40
1:A:2232:TYR:CZ	2:D:73:LEU:HB3	2.56	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:B:2017:ASP:OD1	1:C:2051:LYS:NZ[3_545]	2.18	0.02

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	335/384 (87%)	311 (93%)	23 (7%)	1 (0%)	41	72
1	B	330/384 (86%)	301 (91%)	27 (8%)	2 (1%)	25	59
1	C	325/384 (85%)	300 (92%)	21 (6%)	4 (1%)	13	42
2	D	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
2	E	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
2	F	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	11	39
All	All	1209/1377 (88%)	1118 (92%)	83 (7%)	8 (1%)	22	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	74	ARG
1	B	2055	GLU
1	C	2051	LYS
1	C	2066	GLY
1	C	2046	ASP
1	B	2122	PHE
1	A	2212	THR
1	C	2056	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/351 (90%)	301 (96%)	13 (4%)	30	61
1	B	309/351 (88%)	294 (95%)	15 (5%)	25	56
1	C	304/351 (87%)	296 (97%)	8 (3%)	46	73
2	D	68/68 (100%)	68 (100%)	0	100	100
2	E	68/68 (100%)	68 (100%)	0	100	100
2	F	68/68 (100%)	64 (94%)	4 (6%)	19	48
All	All	1131/1257 (90%)	1091 (96%)	40 (4%)	36	67

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1892	ARG
1	A	1926	LYS
1	A	1977	LYS
1	A	2017	ASP
1	A	2023	GLN
1	A	2032	ARG
1	A	2047	GLU
1	A	2057	ASP
1	A	2059	MET
1	A	2118	TYR
1	A	2187	ASN
1	A	2213	TYR
1	A	2268	PHE
1	B	1892	ARG
1	B	1907	SER
1	B	1923	PHE
1	B	1977	LYS
1	B	2022	SER
1	B	2046	ASP
1	B	2052	ASP
1	B	2058	ASN
1	B	2061	THR

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Mol	Chain	Res	Type
1	B	2062	CYS
1	B	2074	ARG
1	B	2084	LEU
1	B	2122	PHE
1	B	2181	ASN
1	B	2222	ASP
1	C	1892	ARG
1	C	1968	LYS
1	C	2032	ARG
1	C	2059	MET
1	C	2068	LYS
1	C	2070	ARG
1	C	2262	TRP
1	C	2265	ASN
2	F	2	GLN
2	F	54	ARG
2	F	73	LEU
2	F	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2058	ASN
1	B	1941	GLN
1	B	1976	GLN
1	B	2023	GLN
1	B	2181	ASN
1	C	1976	GLN
2	D	2	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AYE	E	101	1,2	3,3,3	0.75	0	1,2,2	2.41	1 (100%)
4	AYE	F	101	-	3,3,3	0.78	0	1,2,2	0.67	0
4	AYE	A	2302	1	3,3,3	0.60	0	1,2,2	2.58	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AYE	E	101	1,2	-	1/1/1/1	-
4	AYE	F	101	-	-	1/1/1/1	-
4	AYE	A	2302	1	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2302	AYE	C1-C2-C3	-2.58	114.19	125.74
4	E	101	AYE	C1-C2-C3	-2.41	114.93	125.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2302	AYE	N1-C1-C2-C3
4	E	101	AYE	N1-C1-C2-C3
4	F	101	AYE	N1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	101	AYE	5	0
4	F	101	AYE	4	0
4	A	2302	AYE	17	0

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	343/384 (89%)	-0.08	8 (2%) 60 40	55, 77, 119, 135	0
1	B	338/384 (88%)	-0.06	10 (2%) 50 29	56, 84, 123, 148	0
1	C	333/384 (86%)	0.33	24 (7%) 15 6	75, 111, 153, 170	0
2	D	75/75 (100%)	-0.28	0 100 100	68, 95, 114, 120	0
2	E	75/75 (100%)	-0.18	0 100 100	72, 104, 123, 132	0
2	F	75/75 (100%)	-0.05	0 100 100	95, 120, 140, 145	0
All	All	1239/1377 (89%)	0.02	42 (3%) 45 24	55, 95, 137, 170	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2178	TYR	4.4
1	B	1926	LYS	3.6
1	C	2067	LYS	3.5
1	C	2267	GLN	3.5
1	C	2051	LYS	3.5
1	C	2056	GLY	3.5
1	C	2014	VAL	3.3
1	C	1926	LYS	3.1
1	A	2268	PHE	3.0
1	B	2223	PHE	3.0
1	A	2224	SER	2.9
1	C	2206	GLY	2.9
1	B	2222	ASP	2.8
1	A	1927	TYR	2.8
1	B	1929	GLU	2.8
1	C	2021	VAL	2.7
1	C	2072	GLU	2.7
1	C	1930	ASP	2.7
1	C	2249	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	2208	MET	2.6
1	C	2226	GLU	2.5
1	C	2225	PHE	2.5
1	A	1968	LYS	2.5
1	A	2067	LYS	2.4
1	C	2068	LYS	2.4
1	C	2066	GLY	2.4
1	C	2059	MET	2.4
1	C	1927	TYR	2.4
1	A	1930	ASP	2.3
1	C	2057	ASP	2.3
1	B	2177	ALA	2.3
1	B	2179	LYS	2.3
1	C	2263	HIS	2.3
1	B	2180	ASN	2.2
1	B	2209	THR	2.2
1	A	2019	GLU	2.2
1	C	2019	GLU	2.2
1	B	2181	ASN	2.2
1	B	2260	TRP	2.1
1	C	2069	VAL	2.1
1	C	2152	GLY	2.0
1	A	2212	THR	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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	AYE	E	101	4/4	0.86	0.31	90,103,113,126	0
4	AYE	A	2302	4/4	0.92	0.48	93,99,102,115	0
4	AYE	F	101	4/4	0.92	0.21	88,89,90,90	0
3	ZN	B	2301	1/1	0.94	0.04	118,118,118,118	0
3	ZN	A	2301	1/1	0.96	0.04	116,116,116,116	0
3	ZN	C	2301	1/1	0.98	0.05	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.