



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:07 AM UTC

PDB ID : 7W3U / pdb_00007w3u
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

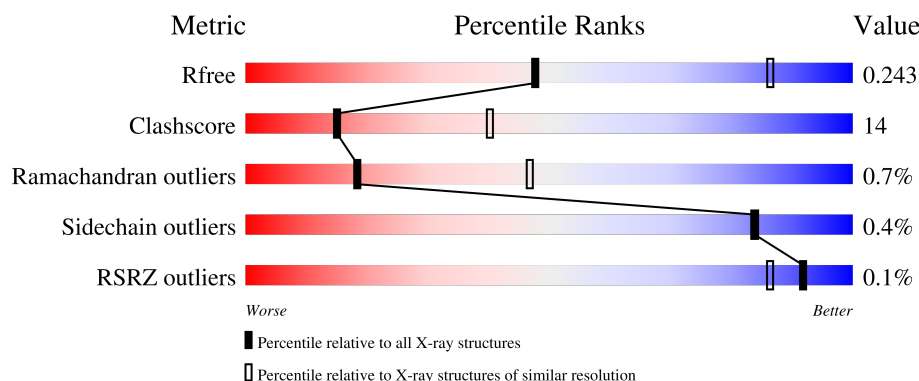
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (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	68% 21% • 11%
1	B	384	63% 24% • 12%
1	C	384	62% 24% • 13%
2	D	75	% 64% 36%
2	E	75	60% 37% •

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Mol	Chain	Length	Quality of chain
2	F	75	 67% 33%

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	B	2302	-	-	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			

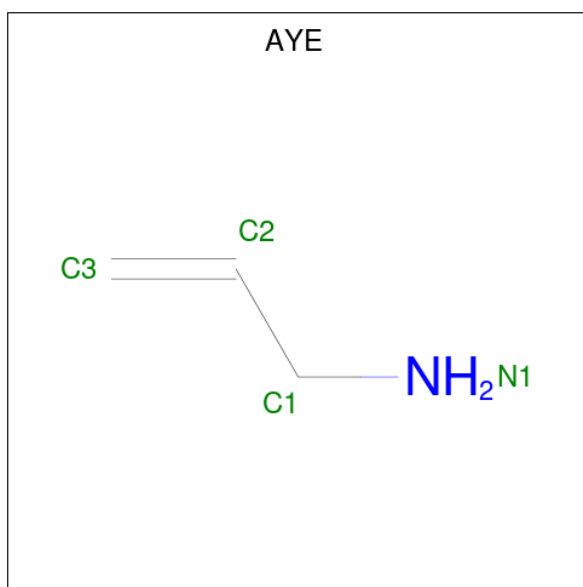
- Molecule 2 is a protein called Polyubiquitin-B.

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 (CCD ID: 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 (CCD ID: AYE) (formula: C₃H₇N).

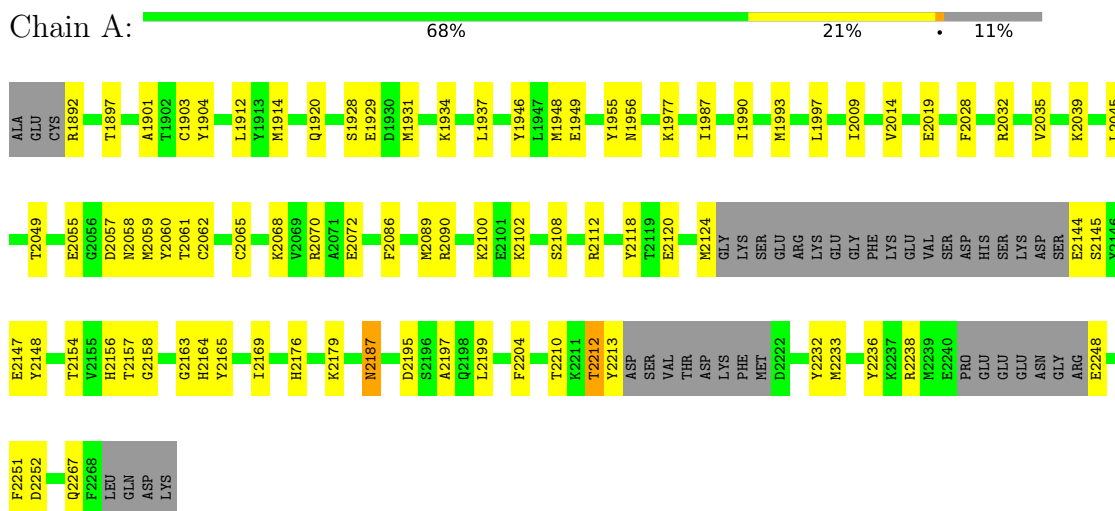


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			4	3	1		
4	B	1	Total	C	N	0	0
			4	3	1		
4	F	1	Total	C	N	0	0
			4	3	1		

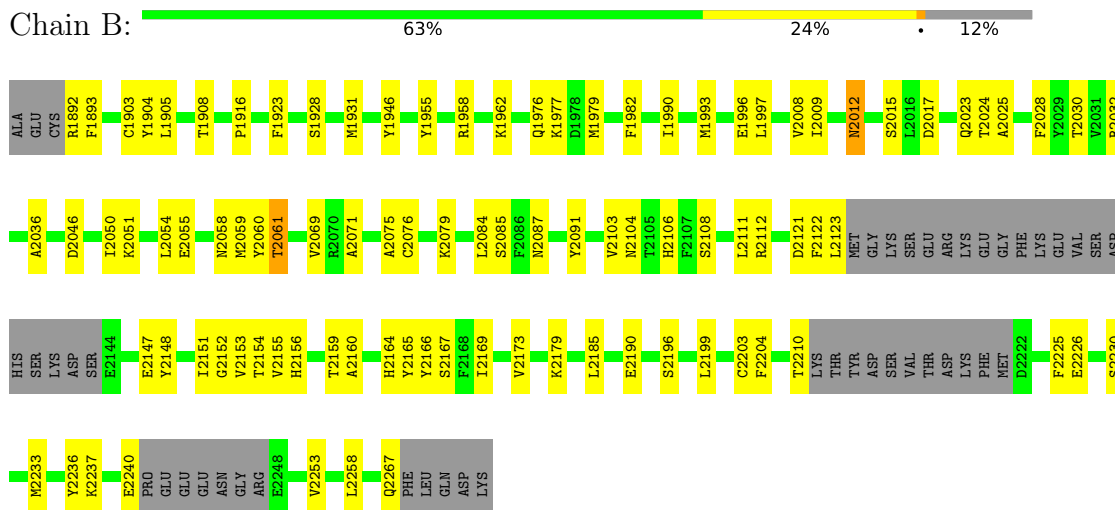
3 Residue-property plots

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 34

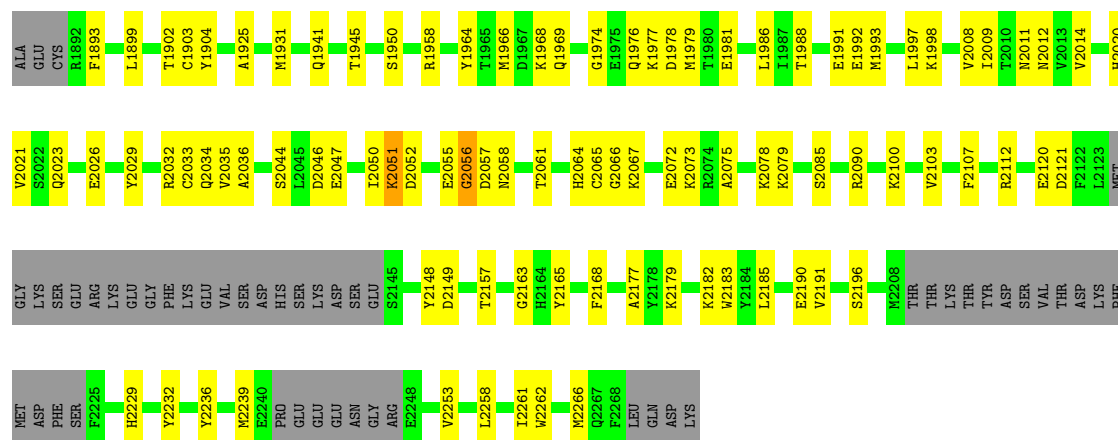


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 34



• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 34





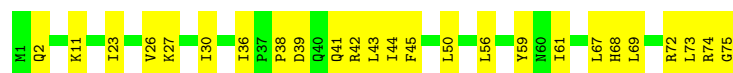
• Molecule 2: Polyubiquitin-B



• Molecule 2: Polyubiquitin-B



• Molecule 2: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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 23.60 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.60-3.13) 89.3 (23.60-3.13)	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 , 0.243	Depositor DCC
R_{free} test set	1988 reflections (7.14%)	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)	0.30 , 45.4	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	0.93	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 [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/2880	0.42	0/3881
1	B	0.16	0/2831	0.40	0/3816
1	C	0.16	0/2794	0.41	0/3765
2	D	0.16	0/603	0.40	0/811
2	E	0.22	0/603	0.45	0/811
2	F	0.14	0/603	0.42	0/811
All	All	0.17	0/10314	0.41	0/13895

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.

There are no bond angle outliers.

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 [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2815	0	2712	76	0
1	B	2768	0	2665	71	1
1	C	2731	0	2636	69	1
2	D	597	0	626	37	0
2	E	597	0	626	33	0
2	F	597	0	626	26	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	18	0
4	B	4	0	4	5	0
4	F	4	0	6	4	0
All	All	10120	0	9907	274	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 14.

All (274) 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
4:A:2302:AYE:H1	2:D:75:GLY:C	1.71	1.15
1:C:1903:CYS:H	4:F:101:AYE:H3A	1.01	1.14
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:B:2302: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2302:AYE:C3	2.12	0.59
1:C:2165:TYR:CE2	2:F:75:GLY:HA3	2.38	0.58
1:A:1990:ILE:HA	1:A:1993:MET:HE2	1.86	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2302: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
1:A:2059:MET:HE3	1:A:2068:LYS:HB2	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1931:MET:HE2	1:A:1993:MET:HB3	1.91	0.52
1:B:1931:MET:HE2	1:B:1993:MET:HB3	1.90	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
1:B:1996:GLU:H	1:B:1996:GLU:CD	2.19	0.50
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:1904:TYR:O	1:B:1908:THR:OG1	2.25	0.50
1:B:2060:TYR:OH	2:E:64:GLU:OE2	2.29	0.50
4:B:2302:AYE:H3	2:E:75:GLY:O	2.12	0.50
1:C:1945:THR:HG23	1:C:2253:VAL:HG11	1.94	0.50
2:E:2:GLN:CD	2:E:14:THR:CG2	2.85	0.50
1:C:1978:ASP:HB2	2:F:72:ARG:HB3	1.93	0.50
1:B:1903:CYS:N	4:B:2302:AYE:H3A	2.16	0.49
1:A:1990:ILE:HA	1:A:1993:MET:HG3	1.95	0.49
1:C:2055:GLU:HG2	1:C:2056:GLY:N	2.26	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
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:1931:MET:HE2	1:C:1993:MET:HB3	1.94	0.48
2:E:2:GLN:CD	2:E:14:THR:HG23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:2187:ASN:ND2	1:A:2187:ASN:C	2.73	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:C:2090:ARG:NH2	1:C:2107:PHE:HB3	2.31	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
1:C:1966:MET:HE1	1:C:1977:LYS:HD2	1.98	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:2032:ARG:HB3	1:A:2089:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1948:MET:HE3	1:A:1949:GLU:OE2	2.17	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
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
1:C:1976:GLN:HB2	2:F:75:GLY:C	2.44	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:22:THR:HG22	2:E:25:ASN:CG	2.44	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
1:B:2155:VAL:HG23	1:B:2230:SER:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1903:CYS:H	4:A:2302:AYE:H3A	1.84	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
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
2:D:2:GLN:O	2:D:2:GLN:HG3	2.20	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:A:1993:MET:HE3	1:A:1997:LEU:HD13	2.03	0.41
1:B:2009:ILE:HG22	1:B:2028:PHE:HD2	1.86	0.41
1:B:2059:MET:HB3	1:B:2059:MET:HE2	1.62	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
1:C:2262:TRP:CD1	1:C:2266:MET:HE3	2.56	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
4:A:2302:AYE:C1	2:D:75:GLY:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

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	335/384 (87%)	311 (93%)	23 (7%)	1 (0%)	36	64
1	B	330/384 (86%)	301 (91%)	27 (8%)	2 (1%)	21	50
1	C	325/384 (85%)	300 (92%)	21 (6%)	4 (1%)	10	34
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%)	9	31
All	All	1209/1377 (88%)	1118 (92%)	83 (7%)	8 (1%)	18	47

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 [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	314/351 (90%)	312 (99%)	2 (1%)	78	80
1	B	309/351 (88%)	307 (99%)	2 (1%)	78	80
1	C	304/351 (87%)	304 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100
2	E	68/68 (100%)	67 (98%)	1 (2%)	57	71
2	F	68/68 (100%)	68 (100%)	0	100	100
All	All	1131/1257 (90%)	1126 (100%)	5 (0%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2057	ASP
1	A	2187	ASN
1	B	2012	ASN
1	B	2061	THR
2	E	3	ILE

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	1920	GLN

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Mol	Chain	Res	Type
1	A	2012	ASN
1	A	2034	GLN
1	A	2058	ASN
1	B	1941	GLN
1	B	1976	GLN
1	B	2023	GLN
1	B	2087	ASN
1	B	2176	HIS
1	B	2181	ASN
1	C	1976	GLN
2	D	2	GLN
2	D	25	ASN
2	E	40	GLN
2	F	68	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 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	A	2302	2,1	3,3,3	0.61	0	2,2,2	3.34	1 (50%)
4	AYE	F	101	2,1	3,3,3	0.72	0	2,2,2	0.98	0
4	AYE	B	2302	2,1	3,3,3	0.75	0	2,2,2	3.00	1 (50%)

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	A	2302	2,1	-	1/1/1/1	-
4	AYE	F	101	2,1	-	1/1/1/1	-
4	AYE	B	2302	2,1	-	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	-4.44	114.19	126.38
4	B	2302	AYE	C1-C2-C3	-4.18	114.93	126.38

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	B	2302	AYE	N1-C1-C2-C3
4	F	101	AYE	N1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2302	AYE	18	0
4	F	101	AYE	4	0
4	B	2302	AYE	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.44	0	100 100	55, 77, 119, 135	0
1	B	338/384 (88%)	-0.37	0	100 100	56, 84, 123, 148	0
1	C	333/384 (86%)	-0.25	0	100 100	75, 111, 153, 170	0
2	D	75/75 (100%)	-0.45	1 (1%)	75 55	68, 95, 114, 120	0
2	E	75/75 (100%)	-0.41	0	100 100	72, 104, 123, 132	0
2	F	75/75 (100%)	-0.25	0	100 100	95, 120, 140, 145	0
All	All	1239/1377 (89%)	-0.36	1 (0%)	92 86	55, 95, 137, 170	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	75	GLY	2.1

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
4	AYE	A	2302	4/4	0.83	0.34	93,99,102,115	0
4	AYE	B	2302	4/4	0.89	0.21	90,103,113,126	0
4	AYE	F	101	4/4	0.91	0.12	88,89,90,90	0
3	ZN	B	2301	1/1	0.96	0.07	118,118,118,118	0
3	ZN	C	2301	1/1	0.98	0.04	147,147,147,147	0
3	ZN	A	2301	1/1	0.99	0.03	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.