Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:28 PM EST

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PDB ID	:	1XM5
Title	:	Crystal structure of metal-dependent hydrolase ybeY from E. coli, Pfam UPF0054
Authors	:	Fedorov, A.A.; Fedorov, E.V.; Shi, W.; Ramagopal, U.A.; Thirumuruhan, R.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-10-01
Resolution	:	2.70 Å(reported)

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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 2.70 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.
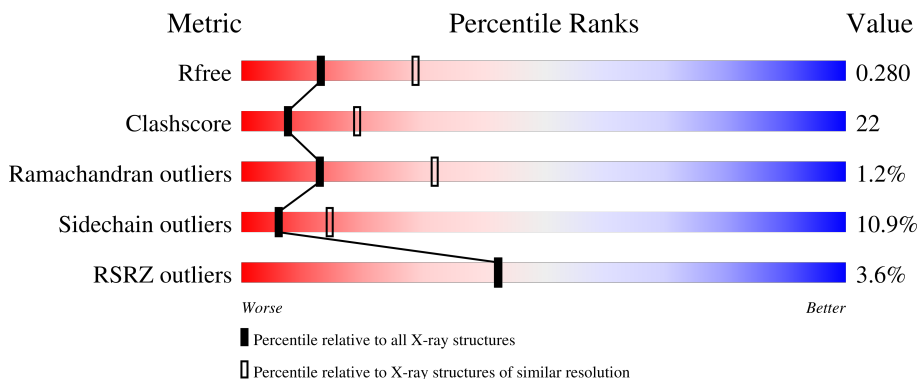
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	3% / 55% / 37% / 6% ·
1	B	155	3% / 57% / 35% / 5% ·
1	C	155	5% / 57% / 34% / 5% 5%
1	D	155	3% / 44% / 47% / 7% ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4781 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 Hypothetical UPF0054 protein ybeY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1201	757	192	244	8			
1	B	152	Total	C	N	O	S	0	0	0
			1201	757	192	244	8			
1	C	148	Total	C	N	O	S	0	0	0
			1174	740	188	239	7			
1	D	152	Total	C	N	O	S	0	0	0
			1201	757	192	244	8			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	A	1	Total	Ni	0	0
			1	1		
2	D	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	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.
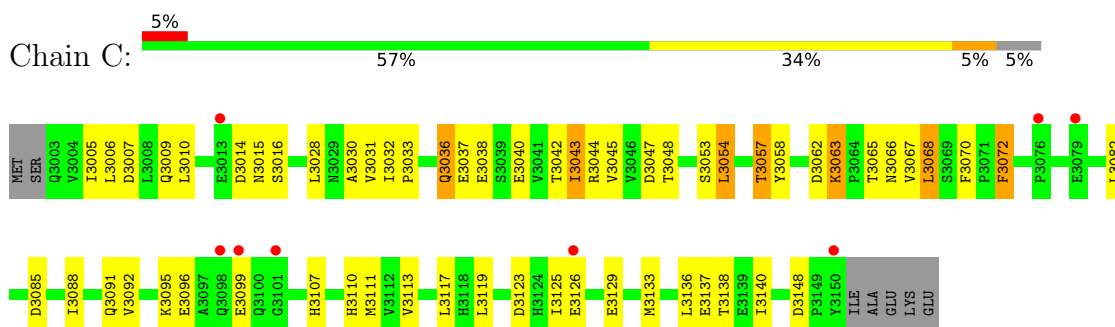
• Molecule 1: Hypothetical UPF0054 protein ybeY
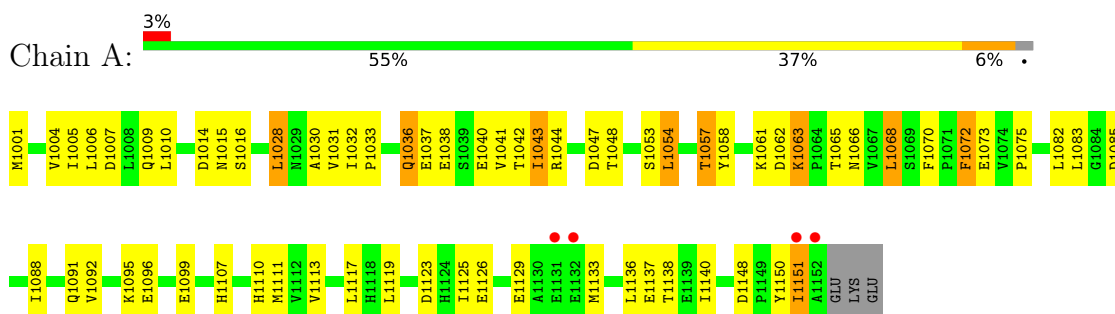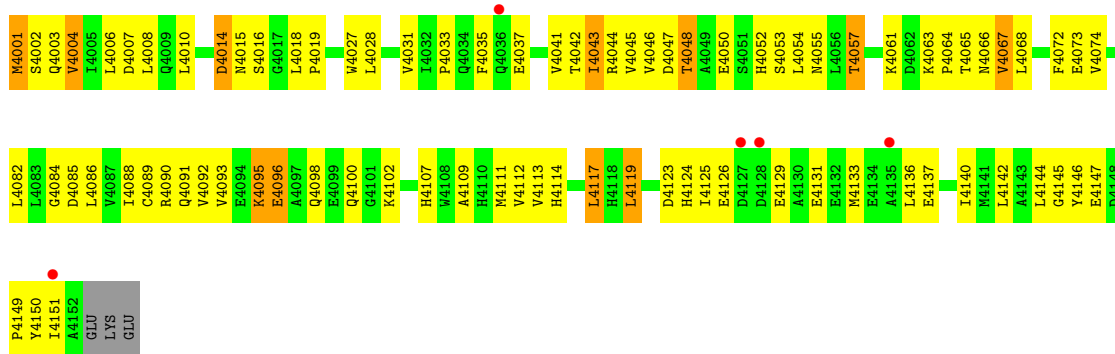

• Molecule 1: Hypothetical UPF0054 protein ybeY
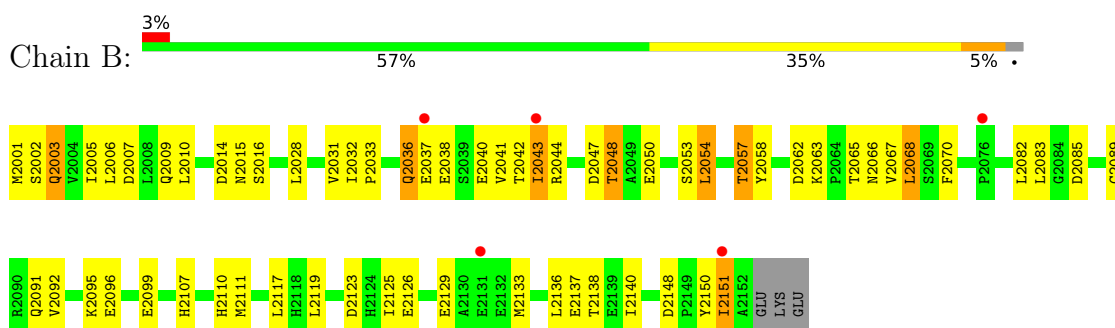
• Molecule 1: Hypothetical UPF0054 protein ybeY

• Molecule 1: Hypothetical UPF0054 protein ybeY

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.07Å 119.61Å 132.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 29.64 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.70) 92.3 (29.64-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.68Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.273 0.241 , 0.280	Depositor DCC
R_{free} test set	1009 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.3	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4781	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.42	0/1226	0.60	0/1667
1	B	0.34	0/1226	0.56	0/1667
1	C	0.34	0/1199	0.57	0/1631
1	D	0.41	0/1226	0.63	0/1667
All	All	0.38	0/4877	0.59	0/6632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1201	0	1146	54	0
1	B	1201	0	1146	53	0
1	C	1174	0	1116	42	0
1	D	1201	0	1146	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	4781	0	4554	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:MET:O	1:A:1037:GLU:HG3	1.70	0.92
1:B:2001:MET:HG2	1:B:2002:SER:H	1.43	0.82
1:A:1057:THR:HB	1:D:4073:GLU:HG3	1.62	0.82
1:C:3031:VAL:HG22	1:C:3140:ILE:HG21	1.66	0.77
1:B:2031:VAL:HG22	1:B:2140:ILE:HG21	1.65	0.77
1:A:1072:PHE:HZ	1:D:4050:GLU:HG3	1.51	0.76
1:D:4006:LEU:HD11	1:D:4043:ILE:HG22	1.68	0.74
1:A:1031:VAL:HG22	1:A:1140:ILE:HG21	1.72	0.72
1:A:1001:MET:C	1:A:1037:GLU:HG3	2.11	0.71
1:A:1072:PHE:CZ	1:D:4050:GLU:HG3	2.25	0.71
1:B:2001:MET:HG2	1:B:2002:SER:N	2.05	0.70
1:A:1136:LEU:O	1:A:1140:ILE:HG12	1.92	0.70
1:B:2136:LEU:O	1:B:2140:ILE:HG12	1.92	0.69
1:B:2005:ILE:HD12	1:B:2005:ILE:H	1.58	0.68
1:C:3136:LEU:O	1:C:3140:ILE:HG12	1.94	0.68
1:D:4043:ILE:HD13	1:D:4043:ILE:C	2.16	0.66
1:A:1005:ILE:H	1:A:1005:ILE:HD12	1.61	0.66
1:C:3005:ILE:H	1:C:3005:ILE:HD12	1.60	0.65
1:A:1053:SER:O	1:A:1057:THR:CG2	2.43	0.65
1:D:4014:ASP:O	1:D:4015:ASN:HB2	1.97	0.65
1:A:1014:ASP:O	1:A:1015:ASN:HB2	1.97	0.64
1:A:1036:GLN:O	1:A:1037:GLU:HB3	1.96	0.64
1:B:2042:THR:HB	1:B:2085:ASP:OD1	1.97	0.64
1:D:4123:ASP:O	1:D:4129:GLU:HG2	1.96	0.64
1:C:3014:ASP:O	1:C:3015:ASN:HB2	1.97	0.64
1:B:2001:MET:CG	1:B:2002:SER:H	2.02	0.64
1:B:2036:GLN:O	1:B:2037:GLU:HB3	1.98	0.64
1:B:2003:GLN:NE2	1:B:2003:GLN:H	1.96	0.63
1:D:4048:THR:HG22	1:D:4064:PRO:HG3	1.79	0.63
1:D:4055:ASN:ND2	1:D:4061:LYS:HB2	2.14	0.62
1:A:1042:THR:HB	1:A:1085:ASP:OD1	2.00	0.61
1:A:1009:GLN:HB2	1:A:1044:ARG:HB3	1.83	0.61
1:B:2006:LEU:HD12	1:B:2007:ASP:N	2.15	0.61
1:B:2053:SER:O	1:B:2057:THR:CG2	2.48	0.61
1:A:1053:SER:O	1:A:1057:THR:HG23	1.99	0.61
1:D:4086:LEU:HD21	1:D:4119:LEU:HD22	1.81	0.61
1:C:3036:GLN:O	1:C:3037:GLU:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2009:GLN:HB2	1:B:2044:ARG:HB3	1.83	0.61
1:C:3009:GLN:HB2	1:C:3044:ARG:HB3	1.83	0.60
1:B:2047:ASP:HA	1:B:2091:GLN:OE1	2.01	0.60
1:C:3005:ILE:N	1:C:3005:ILE:HD12	2.16	0.60
1:D:4042:THR:HB	1:D:4085:ASP:OD1	2.00	0.60
1:D:4001:MET:HG3	1:D:4002:SER:N	2.15	0.60
1:C:3006:LEU:HD12	1:C:3007:ASP:N	2.17	0.60
1:D:4006:LEU:CD1	1:D:4043:ILE:HG22	2.32	0.60
1:A:1006:LEU:HD12	1:A:1007:ASP:N	2.16	0.60
1:A:1075:PRO:HG2	1:D:4052:HIS:CD2	2.37	0.59
1:B:2014:ASP:O	1:B:2015:ASN:HB2	1.99	0.59
1:D:4003:GLN:H	1:D:4003:GLN:NE2	2.01	0.59
1:D:4006:LEU:HD12	1:D:4007:ASP:N	2.17	0.59
1:A:1073:GLU:CD	1:D:4057:THR:HB	2.24	0.58
1:B:2043:ILE:HD13	1:B:2043:ILE:C	2.24	0.57
1:C:3043:ILE:C	1:C:3043:ILE:HD13	2.24	0.57
1:D:4067:VAL:HG13	1:D:4088:ILE:HG12	1.86	0.57
1:A:1043:ILE:HD13	1:A:1043:ILE:C	2.24	0.57
1:C:3042:THR:HB	1:C:3085:ASP:OD1	2.04	0.57
1:B:2125:ILE:HG13	1:B:2126:GLU:HG2	1.87	0.56
1:A:1107:HIS:O	1:A:1111:MET:HG2	2.05	0.56
1:D:4014:ASP:OD2	1:D:4016:SER:HB2	2.04	0.56
1:B:2148:ASP:OD2	1:B:2151:ILE:HB	2.06	0.56
1:B:2053:SER:O	1:B:2057:THR:HG23	2.04	0.56
1:D:4133:MET:O	1:D:4137:GLU:HG3	2.05	0.56
1:A:1125:ILE:HG13	1:A:1126:GLU:HG2	1.87	0.56
1:D:4125:ILE:HG13	1:D:4126:GLU:HG2	1.86	0.56
1:B:2107:HIS:O	1:B:2111:MET:HG2	2.06	0.56
1:C:3053:SER:O	1:C:3057:THR:HG23	2.05	0.56
1:C:3047:ASP:HA	1:C:3091:GLN:OE1	2.06	0.55
1:B:2001:MET:CG	1:B:2002:SER:N	2.68	0.55
1:C:3107:HIS:O	1:C:3111:MET:HG2	2.07	0.55
1:C:3053:SER:O	1:C:3057:THR:CG2	2.54	0.55
1:B:2068:LEU:HB3	1:B:2070:PHE:CE1	2.41	0.55
1:C:3125:ILE:HG13	1:C:3126:GLU:HG2	1.87	0.55
1:B:2005:ILE:HB	1:B:2040:GLU:HB3	1.89	0.55
1:D:4092:VAL:O	1:D:4096:GLU:HG3	2.07	0.55
1:A:1092:VAL:O	1:A:1096:GLU:HG3	2.06	0.54
1:C:3062:ASP:O	1:C:3063:LYS:HB3	2.07	0.54
1:C:3068:LEU:HB3	1:C:3070:PHE:CE1	2.42	0.54
1:A:1062:ASP:O	1:A:1063:LYS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3092:VAL:O	1:C:3096:GLU:HG3	2.08	0.54
1:D:4044:ARG:HG2	1:D:4046:VAL:HG13	1.89	0.54
1:D:4066:ASN:HB2	1:D:4111:MET:SD	2.48	0.54
1:D:4031:VAL:HG22	1:D:4140:ILE:HG21	1.89	0.53
1:A:1068:LEU:HB3	1:A:1070:PHE:CE1	2.43	0.53
1:B:2062:ASP:O	1:B:2063:LYS:HB3	2.09	0.53
1:D:4053:SER:O	1:D:4057:THR:HG23	2.09	0.53
1:D:4096:GLU:OE1	1:D:4107:HIS:HE1	1.92	0.53
1:D:4114:HIS:HE1	1:D:4124:HIS:CD2	2.27	0.53
1:D:4053:SER:O	1:D:4057:THR:CG2	2.56	0.53
1:D:4125:ILE:HG13	1:D:4126:GLU:N	2.23	0.53
1:A:1138:THR:HG23	1:A:1148:ASP:OD1	2.08	0.52
1:A:1053:SER:O	1:A:1057:THR:HG22	2.09	0.52
1:C:3005:ILE:HB	1:C:3040:GLU:HB3	1.91	0.52
1:B:2123:ASP:O	1:B:2129:GLU:HG2	2.09	0.52
1:C:3032:ILE:HB	1:C:3033:PRO:HD3	1.92	0.52
1:D:4008:LEU:HD12	1:D:4043:ILE:HG23	1.92	0.52
1:D:4102:LYS:NZ	1:D:4149:PRO:HA	2.25	0.52
1:A:1005:ILE:HB	1:A:1040:GLU:HB3	1.92	0.51
1:A:1032:ILE:HB	1:A:1033:PRO:HD3	1.92	0.51
1:D:4008:LEU:CD1	1:D:4043:ILE:HG23	2.40	0.51
1:B:2032:ILE:HB	1:B:2033:PRO:HD3	1.93	0.51
1:B:2041:VAL:HG12	1:B:2083:LEU:HB2	1.93	0.51
1:A:1005:ILE:N	1:A:1005:ILE:HD12	2.24	0.51
1:B:2092:VAL:O	1:B:2096:GLU:HG3	2.11	0.51
1:C:3138:THR:HG23	1:C:3148:ASP:OD1	2.11	0.50
1:D:4031:VAL:CG2	1:D:4113:VAL:HG22	2.41	0.50
1:C:3110:HIS:HE1	1:C:3137:GLU:OE1	1.94	0.50
1:D:4006:LEU:HD12	1:D:4007:ASP:H	1.76	0.50
1:A:1037:GLU:HG2	1:A:1038:GLU:HG3	1.93	0.50
1:D:4089:CYS:O	1:D:4093:VAL:HG23	2.12	0.49
1:A:1110:HIS:HE1	1:A:1137:GLU:OE1	1.94	0.49
1:B:2053:SER:O	1:B:2057:THR:HG22	2.12	0.49
1:C:3123:ASP:O	1:C:3129:GLU:HG2	2.14	0.48
1:D:4113:VAL:O	1:D:4117:LEU:HD22	2.13	0.48
1:D:4057:THR:OG1	1:D:4057:THR:O	2.31	0.48
1:B:2138:THR:HG23	1:B:2148:ASP:OD1	2.13	0.48
1:A:1006:LEU:HD11	1:A:1043:ILE:CG2	2.43	0.48
1:C:3006:LEU:HD11	1:C:3043:ILE:CG2	2.43	0.48
1:B:2125:ILE:HG13	1:B:2126:GLU:N	2.29	0.48
1:D:4102:LYS:HZ1	1:D:4149:PRO:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3010:LEU:HB3	1:C:3015:ASN:OD1	2.14	0.47
1:D:4033:PRO:HG2	1:D:4035:PHE:CZ	2.49	0.47
1:D:4006:LEU:HD11	1:D:4043:ILE:CG2	2.39	0.47
1:B:2010:LEU:HB3	1:B:2015:ASN:OD1	2.14	0.47
1:D:4027:TRP:CB	1:D:4112:VAL:HG21	2.45	0.47
1:B:2006:LEU:HD12	1:B:2007:ASP:H	1.79	0.47
1:A:1006:LEU:HD12	1:A:1007:ASP:H	1.80	0.47
1:A:1036:GLN:HE21	1:A:1036:GLN:HB3	1.55	0.47
1:B:2110:HIS:HE1	1:B:2137:GLU:OE1	1.97	0.47
1:B:2133:MET:O	1:B:2137:GLU:HG3	2.15	0.47
1:B:2006:LEU:HD11	1:B:2043:ILE:CG2	2.45	0.46
1:C:3006:LEU:HD12	1:C:3007:ASP:H	1.79	0.46
1:C:3006:LEU:CD1	1:C:3043:ILE:HG22	2.45	0.46
1:D:4114:HIS:CE1	1:D:4124:HIS:CD2	3.04	0.46
1:A:1125:ILE:HG13	1:A:1126:GLU:N	2.30	0.46
1:A:1047:ASP:HA	1:A:1091:GLN:OE1	2.15	0.46
1:C:3125:ILE:HG13	1:C:3126:GLU:N	2.30	0.46
1:A:1014:ASP:OD2	1:A:1016:SER:HB2	2.16	0.46
1:C:3014:ASP:OD2	1:C:3016:SER:HB2	2.16	0.46
1:A:1123:ASP:O	1:A:1129:GLU:HG2	2.15	0.46
1:C:3095:LYS:O	1:C:3099:GLU:HG3	2.16	0.46
1:D:4096:GLU:O	1:D:4100:GLN:HG3	2.16	0.45
1:D:4095:LYS:O	1:D:4096:GLU:C	2.55	0.45
1:B:2014:ASP:OD2	1:B:2016:SER:HB2	2.16	0.45
1:B:2006:LEU:CD1	1:B:2043:ILE:HG22	2.47	0.45
1:D:4123:ASP:OD2	1:D:4125:ILE:HG23	2.17	0.45
1:B:2005:ILE:HD12	1:B:2005:ILE:N	2.27	0.45
1:D:4109:ALA:O	1:D:4112:VAL:HG22	2.16	0.45
1:A:1006:LEU:CD1	1:A:1043:ILE:HG22	2.46	0.45
1:A:1010:LEU:HB3	1:A:1015:ASN:OD1	2.17	0.45
1:B:2037:GLU:HG2	1:B:2038:GLU:HG3	1.98	0.45
1:A:1004:VAL:HG23	1:A:1033:PRO:HG3	1.98	0.44
1:B:2050:GLU:HG3	1:C:3072:PHE:CZ	2.52	0.44
1:D:4095:LYS:O	1:D:4098:GLN:N	2.50	0.44
1:D:4031:VAL:HG21	1:D:4113:VAL:HG22	1.99	0.44
1:D:4142:LEU:O	1:D:4145:GLY:N	2.51	0.44
1:D:4090:ARG:HG3	1:D:4091:GLN:N	2.32	0.44
1:A:1150:TYR:O	1:A:1151:ILE:HB	2.18	0.44
1:D:4016:SER:O	1:D:4090:ARG:NH2	2.36	0.43
1:D:4142:LEU:HA	1:D:4146:TYR:O	2.18	0.43
1:B:2036:GLN:HE21	1:B:2036:GLN:HB3	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4027:TRP:HB3	1:D:4112:VAL:HG21	2.00	0.43
1:B:2095:LYS:O	1:B:2099:GLU:HG3	2.19	0.43
1:A:1072:PHE:CZ	1:D:4050:GLU:HA	2.53	0.43
1:C:3037:GLU:HG2	1:C:3038:GLU:HG3	1.99	0.43
1:C:3045:VAL:HA	1:C:3088:ILE:O	2.19	0.43
1:B:2048:THR:HG23	1:B:2091:GLN:HB2	2.01	0.43
1:D:4047:ASP:HB3	1:D:4091:GLN:HE22	1.83	0.43
1:A:1031:VAL:CG2	1:A:1113:VAL:HG22	2.48	0.42
1:C:3030:ALA:O	1:C:3140:ILE:HD12	2.19	0.42
1:C:3031:VAL:HG21	1:C:3113:VAL:HG22	2.01	0.42
1:A:1133:MET:O	1:A:1137:GLU:HG3	2.19	0.42
1:A:1061:LYS:HE2	1:C:3125:ILE:HD11	2.01	0.42
1:B:2050:GLU:HG3	1:C:3072:PHE:CE2	2.54	0.42
1:C:3031:VAL:CG2	1:C:3113:VAL:HG22	2.49	0.42
1:C:3133:MET:O	1:C:3137:GLU:HG3	2.19	0.42
1:B:2089:CYS:SG	1:B:2092:VAL:HG23	2.60	0.42
1:B:2150:TYR:O	1:B:2151:ILE:C	2.57	0.42
1:B:2006:LEU:HD11	1:B:2043:ILE:HG22	2.02	0.42
1:A:1030:ALA:O	1:A:1140:ILE:HD12	2.20	0.41
1:B:2043:ILE:HD13	1:B:2043:ILE:O	2.20	0.41
1:D:4150:TYR:O	1:D:4151:ILE:C	2.57	0.41
1:A:1028:LEU:HD12	1:A:1028:LEU:HA	1.88	0.41
1:D:4114:HIS:CE1	1:D:4133:MET:HE1	2.55	0.41
1:A:1066:ASN:O	1:A:1088:ILE:HA	2.20	0.41
1:B:2054:LEU:HD12	1:B:2058:TYR:CE1	2.55	0.41
1:D:4019:PRO:HB3	1:D:4027:TRP:CH2	2.55	0.41
1:A:1095:LYS:O	1:A:1099:GLU:HG3	2.21	0.41
1:B:2068:LEU:HA	1:B:2068:LEU:HD12	1.92	0.41
1:D:4018:LEU:HD22	1:D:4045:VAL:HG11	2.02	0.41
1:D:4043:ILE:C	1:D:4043:ILE:CD1	2.88	0.41
1:B:2066:ASN:HB2	1:B:2111:MET:SD	2.61	0.41
1:B:2066:ASN:OD1	1:B:2067:VAL:N	2.54	0.41
1:A:1054:LEU:HD12	1:A:1058:TYR:HE1	1.86	0.41
1:B:2003:GLN:N	1:B:2003:GLN:NE2	2.68	0.41
1:D:4003:GLN:HG2	1:D:4004:VAL:HG23	2.03	0.41
1:C:3054:LEU:HD12	1:C:3058:TYR:CE1	2.56	0.40
1:C:3068:LEU:HD12	1:C:3068:LEU:HA	1.93	0.40
1:D:4002:SER:HB2	1:D:4003:GLN:NE2	2.36	0.40
1:A:1054:LEU:HD12	1:A:1058:TYR:CE1	2.56	0.40
1:A:1041:VAL:HG12	1:A:1083:LEU:HB2	2.04	0.40
1:A:1031:VAL:HG21	1:A:1113:VAL:HG22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:GLN:O	1:A:1038:GLU:N	2.54	0.40
1:D:4072:PHE:CD2	1:D:4084:GLY:HA2	2.57	0.40
1:C:3066:ASN:OD1	1:C:3067:VAL:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/155 (97%)	136 (91%)	12 (8%)	2 (1%)	12	30
1	B	150/155 (97%)	136 (91%)	13 (9%)	1 (1%)	22	46
1	C	146/155 (94%)	133 (91%)	12 (8%)	1 (1%)	22	46
1	D	150/155 (97%)	131 (87%)	16 (11%)	3 (2%)	7	19
All	All	596/620 (96%)	536 (90%)	53 (9%)	7 (1%)	13	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2151	ILE
1	D	4095	LYS
1	D	4014	ASP
1	D	4096	GLU
1	A	1151	ILE
1	C	3063	LYS
1	A	1063	LYS

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	134/137 (98%)	122 (91%)	12 (9%)	9	22
1	B	134/137 (98%)	122 (91%)	12 (9%)	9	22
1	C	131/137 (96%)	119 (91%)	12 (9%)	9	21
1	D	134/137 (98%)	112 (84%)	22 (16%)	2	6
All	All	533/548 (97%)	475 (89%)	58 (11%)	6	14

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	LEU
1	A	1036	GLN
1	A	1043	ILE
1	A	1048	THR
1	A	1054	LEU
1	A	1057	THR
1	A	1065	THR
1	A	1068	LEU
1	A	1072	PHE
1	A	1082	LEU
1	A	1117	LEU
1	A	1119	LEU
1	B	2003	GLN
1	B	2028	LEU
1	B	2036	GLN
1	B	2043	ILE
1	B	2048	THR
1	B	2054	LEU
1	B	2057	THR
1	B	2065	THR
1	B	2068	LEU
1	B	2082	LEU
1	B	2117	LEU
1	B	2119	LEU
1	C	3028	LEU
1	C	3036	GLN
1	C	3043	ILE
1	C	3048	THR

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Mol	Chain	Res	Type
1	C	3054	LEU
1	C	3057	THR
1	C	3065	THR
1	C	3068	LEU
1	C	3072	PHE
1	C	3082	LEU
1	C	3117	LEU
1	C	3119	LEU
1	D	4001	MET
1	D	4004	VAL
1	D	4010	LEU
1	D	4028	LEU
1	D	4037	GLU
1	D	4041	VAL
1	D	4043	ILE
1	D	4048	THR
1	D	4054	LEU
1	D	4057	THR
1	D	4063	LYS
1	D	4065	THR
1	D	4067	VAL
1	D	4068	LEU
1	D	4074	VAL
1	D	4082	LEU
1	D	4117	LEU
1	D	4119	LEU
1	D	4131	GLU
1	D	4136	LEU
1	D	4144	LEU
1	D	4147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1003	GLN
1	A	1034	GLN
1	A	1036	GLN
1	A	1107	HIS
1	A	1110	HIS
1	B	2003	GLN
1	B	2034	GLN
1	B	2036	GLN

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Mol	Chain	Res	Type
1	B	2107	HIS
1	B	2110	HIS
1	C	3034	GLN
1	C	3036	GLN
1	C	3107	HIS
1	C	3110	HIS
1	D	4003	GLN
1	D	4052	HIS
1	D	4107	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 monosaccharides 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	152/155 (98%)	0.04	4 (2%)	56	57	26, 51, 108, 131	0
1	B	152/155 (98%)	0.28	5 (3%)	46	46	39, 73, 122, 145	0
1	C	148/155 (95%)	0.41	8 (5%)	25	24	46, 88, 128, 146	0
1	D	152/155 (98%)	0.08	5 (3%)	46	46	29, 61, 115, 145	0
All	All	604/620 (97%)	0.20	22 (3%)	42	42	26, 70, 123, 146	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1151	ILE	4.5
1	C	3101	GLY	3.8
1	A	1131	GLU	3.1
1	A	1152	ALA	3.1
1	B	2043	ILE	3.1
1	B	2151	ILE	3.0
1	C	3126	GLU	2.8
1	D	4036	GLN	2.5
1	C	3098	GLN	2.5
1	D	4128	ASP	2.5
1	C	3079	GLU	2.4
1	D	4135	ALA	2.4
1	C	3150	TYR	2.4
1	B	2131	GLU	2.4
1	B	2076	PRO	2.4
1	D	4151	ILE	2.4
1	C	3099	GLU	2.3
1	B	2037	GLU	2.2
1	A	1132	GLU	2.2
1	C	3076	PRO	2.2
1	D	4127	ASP	2.2
1	C	3013	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NI	D	5004	1/1	0.97	0.24	54,54,54,54	0
2	NI	B	5002	1/1	0.98	0.20	48,48,48,48	0
2	NI	C	5003	1/1	0.99	0.20	61,61,61,61	0
2	NI	A	5001	1/1	0.99	0.22	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.