WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 03:08 PM EDT

PDB ID	:	3UYW
Title	:	Crystal structures of globular head of 2009 pandemic H1N1 hemagglutinin
Authors	:	Xuan, C.L.; Shi, Y.; Qi, J.X.; Xiao, H.X.; Gao, G.F.
Deposited on	:	2011-12-06
Resolution	:	1.90 Å(reported)

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	:	2.36
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)	:	2.36
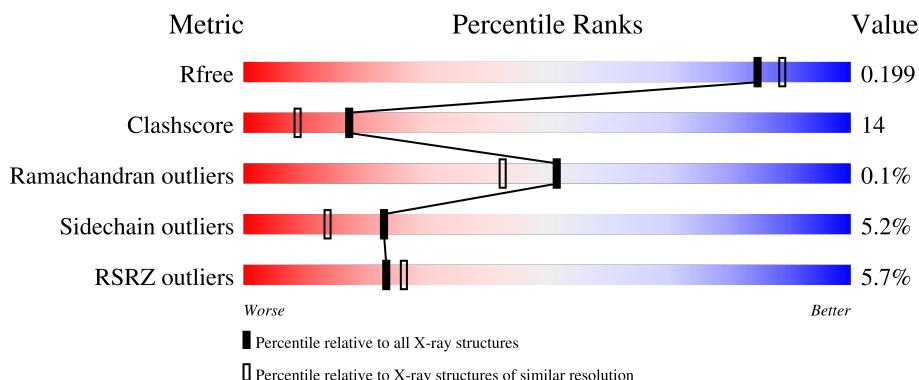
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
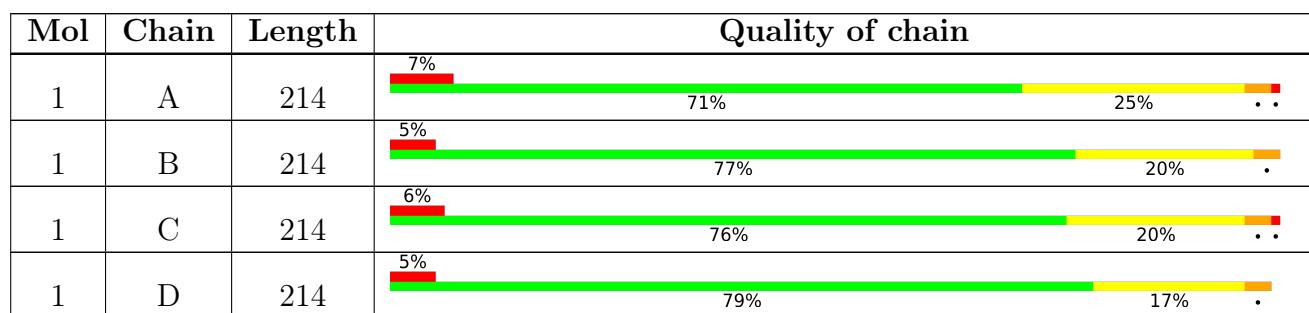
The reported resolution of this entry is 1.90 Å.

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	Percentile Ranks	Value
Rfree		0.199
Clashscore		14
Ramachandran outliers		0.1%
Sidechain outliers		5.2%
RSRZ outliers		5.7%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	214	7% / 71% / 25% / ..
1	B	214	5% / 77% / 20% / .
1	C	214	6% / 76% / 20% / ..
1	D	214	5% / 79% / 17% / .

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2 Entry composition ⓘ
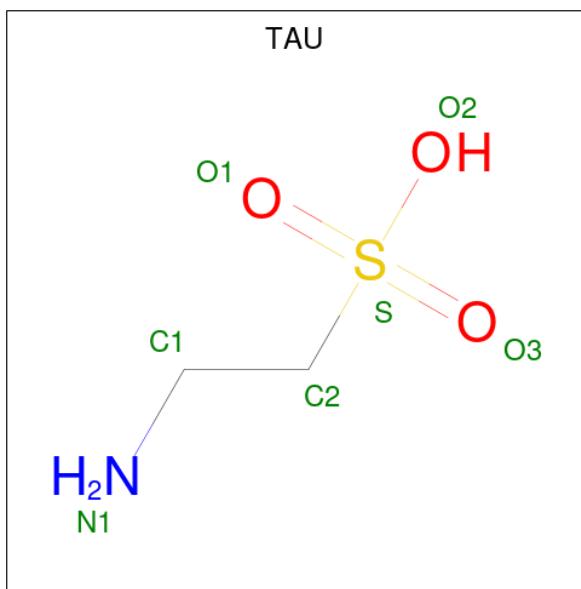
There are 3 unique types of molecules in this entry. The entry contains 7664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total 1703	C 1087	N 287	O 323	S 6	0	0	0
1	B	214	Total 1709	C 1090	N 288	O 325	S 6	0	1	0
1	C	214	Total 1708	C 1089	N 288	O 325	S 6	0	1	0
1	D	214	Total 1709	C 1090	N 288	O 325	S 6	0	1	0

- Molecule 2 is 2-AMINOETHANESULFONIC ACID (three-letter code: TAU) (formula: $C_2H_7NO_3S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 7	C 2	N 1	O 3	S 1	0	0
2	C	1	Total 7	C 2	N 1	O 3	S 1	0	0
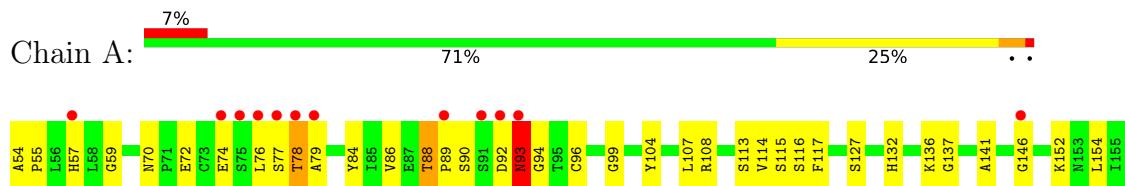
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0
3	B	203	Total 203	O 203	0	0
3	C	202	Total 202	O 202	0	0
3	D	219	Total 219	O 219	0	0
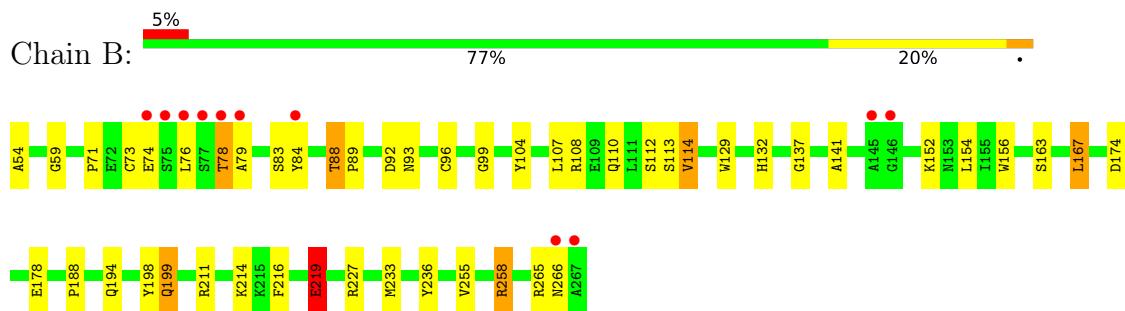
3 Residue-property plots ⓘ

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.
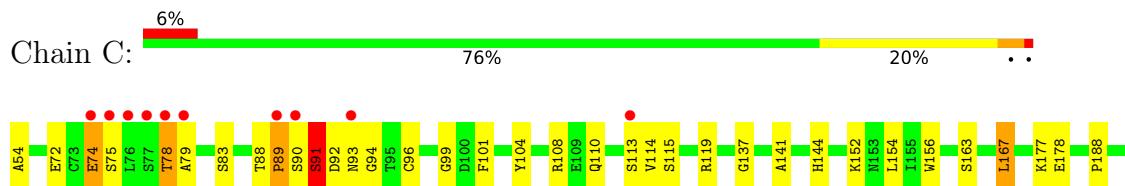
- Molecule 1: Hemagglutinin
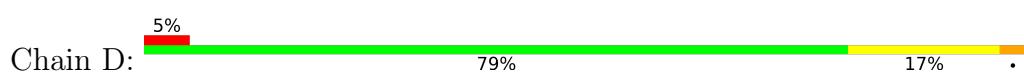
Chain A:

- Molecule 1: Hemagglutinin

Chain B:

- Molecule 1: Hemagglutinin

Chain C:

- Molecule 1: Hemagglutinin

Chain D:

A54 K60 E72 C73 E74 S75 L76 S77 T78 A79 S80 S83 Y84 G99 D100 F101 Y104 R108 E109 S112 S113 V114 S115 S116 F117 E118 R119 G137 A145 G146 K152 W156 N162 S163 L167 P188 Q194 Q195 Y198 Q199 R211 K214

E219 R223 M233 Y236 E241 E249 R258 N266 A267
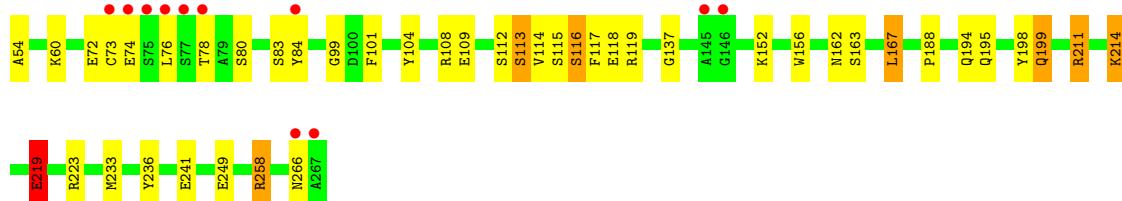
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.67Å 65.92Å 79.48Å 94.46° 89.97° 94.88°	Depositor
Resolution (Å)	35.13 – 1.90 38.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.13-1.90) 97.1 (38.53-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.94 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.184 , 0.198 0.185 , 0.199	Depositor DCC
R_{free} test set	3015 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7664	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4394e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: TAU

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	0.71	2/1753 (0.1%)	0.69	3/2380 (0.1%)
1	B	0.79	7/1759 (0.4%)	0.63	1/2388 (0.0%)
1	C	0.75	2/1758 (0.1%)	0.79	8/2386 (0.3%)
1	D	0.79	3/1759 (0.2%)	0.73	5/2388 (0.2%)
All	All	0.76	14/7029 (0.2%)	0.71	17/9542 (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	3
1	C	0	1
All	All	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	GLU	CB-CG	-6.93	1.39	1.52
1	A	219	GLU	CB-CG	-6.81	1.39	1.52
1	D	249	GLU	CB-CG	-5.69	1.41	1.52
1	D	113	SER	CB-OG	-5.63	1.34	1.42
1	B	258	ARG	CB-CG	-5.47	1.37	1.52
1	B	178	GLU	CB-CG	-5.34	1.42	1.52
1	B	59	GLY	C-O	-5.32	1.15	1.23
1	B	219	GLU	CG-CD	-5.16	1.44	1.51
1	B	114	VAL	CB-CG2	-5.11	1.42	1.52
1	C	74	GLU	CG-CD	5.11	1.59	1.51
1	B	258	ARG	CG-CD	-5.10	1.39	1.51
1	D	219	GLU	CG-CD	-5.10	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	GLU	CB-CG	-5.07	1.42	1.52
1	A	116	SER	CB-OG	-5.02	1.35	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	D	119	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	C	91	SER	N-CA-CB	-9.67	96.00	110.50
1	C	258	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	D	119	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	B	199	GLN	CB-CA-C	-8.78	92.84	110.40
1	A	258	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	C	258	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	167	LEU	CA-CB-CG	7.87	133.40	115.30
1	C	89	PRO	CB-CA-C	-7.39	93.53	112.00
1	C	119	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	A	199	GLN	CB-CA-C	-6.75	96.89	110.40
1	C	265	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	119	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	D	258	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	199	GLN	CB-CA-C	-6.46	97.48	110.40
1	D	199	GLN	CB-CA-C	-5.34	99.72	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	PRO	Mainchain,Peptide
1	A	93	ASN	Peptide
1	C	91	SER	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	1703	0	1637	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1709	0	1641	38	0
1	C	1708	0	1636	47	0
1	D	1709	0	1641	38	0
2	A	7	0	6	1	0
2	C	7	0	6	0	0
3	A	197	0	0	21	0
3	B	203	0	0	11	0
3	C	202	0	0	9	0
3	D	219	0	0	17	0
All	All	7664	0	6567	185	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 14.

All (185) 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:211:ARG:NH2	1:A:241:GLU:CG	1.73	1.48
1:A:59:GLY:O	1:A:88:THR:CG2	1.79	1.28
1:A:211:ARG:NH2	1:A:241:GLU:HG3	1.35	1.26
1:A:92:ASP:O	1:A:94:GLY:N	1.69	1.25
1:A:211:ARG:HH21	1:A:241:GLU:CD	1.39	1.25
1:A:59:GLY:O	1:A:88:THR:HG23	1.38	1.19
1:D:54:ALA:N	3:D:605:HOH:O	1.82	1.12
1:C:54:ALA:N	3:C:587:HOH:O	1.81	1.11
1:B:54:ALA:N	3:B:693:HOH:O	1.83	1.08
1:D:83:SER:CB	3:D:644:HOH:O	1.99	1.08
1:D:72:GLU:HG3	3:D:779:HOH:O	1.55	1.04
1:B:110:GLN:NE2	3:B:776:HOH:O	1.83	1.03
1:A:211:ARG:NH2	1:A:241:GLU:HG2	1.75	1.01
1:C:74:GLU:CG	1:C:75:SER:H	1.71	1.01
1:A:211:ARG:HH21	1:A:241:GLU:CG	1.48	1.00
1:C:74:GLU:HG2	1:C:75:SER:N	1.70	1.00
1:C:74:GLU:HG2	1:C:75:SER:H	0.86	1.00
2:A:1:TAU:N1	3:A:571:HOH:O	1.95	0.99
1:C:239:LEU:HD11	1:C:265:ARG:HH22	1.27	0.99
1:A:76:LEU:O	3:A:586:HOH:O	1.81	0.98
1:B:199:GLN:O	1:B:199:GLN:HG3	1.63	0.97
1:C:211:ARG:CZ	1:C:241:GLU:HG3	1.94	0.97
1:C:163:SER:O	3:C:555:HOH:O	1.81	0.97
1:D:83:SER:C	3:D:644:HOH:O	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HH22	1:A:241:GLU:CG	1.75	0.92
1:A:88:THR:O	3:A:703:HOH:O	1.88	0.92
1:A:211:ARG:NH2	1:A:241:GLU:OE2	2.03	0.92
1:A:168:SER:OG	3:A:327:HOH:O	1.87	0.92
1:A:59:GLY:O	1:A:88:THR:HG21	1.68	0.90
1:B:163:SER:HB2	3:B:569:HOH:O	1.72	0.89
1:A:88:THR:C	3:A:703:HOH:O	2.11	0.88
1:A:211:ARG:HH22	1:A:241:GLU:HG2	1.30	0.87
1:D:83:SER:OG	3:D:644:HOH:O	1.91	0.86
1:A:200:ASN:OD1	3:A:598:HOH:O	1.94	0.85
1:D:73:CYS:O	3:D:406:HOH:O	1.94	0.84
1:D:84:TYR:N	3:D:644:HOH:O	2.11	0.83
1:C:91:SER:HA	1:C:94:GLY:H	1.41	0.82
1:A:78:THR:N	3:A:586:HOH:O	2.13	0.79
1:A:211:ARG:CZ	1:A:241:GLU:HG3	2.13	0.79
1:C:91:SER:HA	1:C:94:GLY:N	1.98	0.79
1:B:219:GLU:O	1:B:219:GLU:HG3	1.83	0.78
1:A:136:LYS:NZ	3:A:582:HOH:O	1.99	0.77
1:C:83:SER:O	3:C:338:HOH:O	2.03	0.77
1:C:195:GLN:OE1	3:C:524:HOH:O	2.04	0.75
1:C:239:LEU:HD11	1:C:265:ARG:NH2	2.03	0.73
1:C:239:LEU:CD1	1:C:265:ARG:HH22	2.01	0.73
1:D:219:GLU:O	1:D:219:GLU:HG3	1.85	0.72
1:A:199:GLN:O	1:A:199:GLN:HG3	1.90	0.71
1:C:144:HIS:CD2	3:C:758:HOH:O	2.43	0.71
1:B:199:GLN:O	1:B:199:GLN:CG	2.37	0.69
1:A:219:GLU:HG3	1:A:219:GLU:O	1.91	0.69
1:D:84:TYR:CD2	3:D:644:HOH:O	2.48	0.67
1:C:90:SER:O	3:C:695:HOH:O	2.12	0.66
1:D:118:GLU:OE2	3:D:547:HOH:O	2.14	0.66
1:A:127:SER:O	3:A:817:HOH:O	2.13	0.66
1:C:91:SER:OG	1:C:94:GLY:HA3	1.95	0.65
1:C:199:GLN:O	1:C:199:GLN:HG3	1.95	0.65
1:A:77:SER:HA	3:A:586:HOH:O	1.95	0.65
1:A:264:GLU:OE1	3:A:765:HOH:O	2.14	0.65
1:C:219:GLU:OE2	3:C:764:HOH:O	2.15	0.65
1:D:109:GLU:HG2	3:D:646:HOH:O	1.97	0.64
1:A:57:HIS:ND1	3:A:399:HOH:O	2.30	0.64
1:A:188:PRO:HG2	1:A:194:GLN:HE21	1.62	0.64
1:A:57:HIS:CE1	1:A:86:VAL:HG11	2.33	0.63
1:B:132:HIS:HD2	3:B:395:HOH:O	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PRO:HG2	1:B:194:GLN:HE21	1.64	0.62
1:C:219:GLU:O	1:C:219:GLU:HG3	2.00	0.61
1:D:83:SER:HB2	3:D:644:HOH:O	1.84	0.61
1:A:265:ARG:HG2	1:A:265:ARG:HH11	1.65	0.60
1:D:188:PRO:HG2	1:D:194:GLN:HE21	1.67	0.60
1:C:188:PRO:HG2	1:C:194:GLN:HE21	1.66	0.60
1:B:174:ASP:OD1	3:B:392:HOH:O	2.15	0.59
1:A:55:PRO:HB3	1:A:84:TYR:CZ	2.38	0.59
1:C:88:THR:HG22	1:C:89:PRO:N	2.18	0.59
1:D:113:SER:OG	1:D:266:ASN:HB2	2.03	0.58
1:B:110:GLN:HB2	3:B:776:HOH:O	2.02	0.58
1:A:92:ASP:OD1	1:A:93:ASN:N	2.37	0.58
1:B:129:TRP:O	3:B:288:HOH:O	2.17	0.57
1:D:84:TYR:HA	1:D:112:SER:O	2.04	0.56
1:D:163:SER:HB2	3:D:671:HOH:O	2.04	0.56
1:A:214:LYS:HG2	1:A:216:PHE:CZ	2.41	0.55
1:C:178:GLU:OE1	1:C:265:ARG:NH1	2.39	0.55
1:A:90:SER:HB2	1:A:93:ASN:HB2	1.88	0.55
1:C:214:LYS:HG2	1:C:216:PHE:CZ	2.41	0.55
1:D:211:ARG:HH21	1:D:241:GLU:CG	2.20	0.54
1:A:188:PRO:HG2	1:A:194:GLN:NE2	2.22	0.54
1:B:188:PRO:HG2	1:B:194:GLN:NE2	2.23	0.54
1:A:72:GLU:CG	3:A:754:HOH:O	2.55	0.54
1:B:214:LYS:HE3	1:B:216:PHE:CE2	2.43	0.54
1:C:211:ARG:CZ	1:C:241:GLU:CG	2.65	0.53
1:D:83:SER:CA	3:D:644:HOH:O	2.32	0.53
1:A:99:GLY:HA3	1:A:233:MET:O	2.08	0.53
1:A:211:ARG:NH2	1:A:241:GLU:CD	2.17	0.52
1:B:219:GLU:OE1	1:C:236:TYR:OH	2.27	0.52
1:D:188:PRO:HG2	1:D:194:GLN:NE2	2.24	0.52
1:D:219:GLU:HG2	1:D:223:ARG:NH2	2.25	0.52
1:B:99:GLY:HA3	1:B:233:MET:O	2.10	0.52
1:D:114:VAL:HG11	1:D:117:PHE:HB2	1.91	0.52
1:A:77:SER:CA	3:A:586:HOH:O	2.57	0.51
1:B:167:LEU:C	1:B:167:LEU:HD12	2.31	0.51
1:B:211:ARG:O	3:B:433:HOH:O	2.19	0.51
1:C:188:PRO:HG2	1:C:194:GLN:NE2	2.24	0.51
1:A:72:GLU:HB3	1:A:93:ASN:ND2	2.25	0.51
1:B:227:ARG:HD3	3:B:607:HOH:O	2.11	0.50
1:B:236:TYR:OH	1:C:219:GLU:OE1	2.28	0.50
1:D:211:ARG:HH21	1:D:241:GLU:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:TYR:CE2	1:D:108:ARG:HD2	2.47	0.50
1:D:199:GLN:HG3	1:D:199:GLN:O	2.10	0.50
1:B:104:TYR:CE2	1:B:108:ARG:HD2	2.46	0.50
1:A:198:TYR:O	1:A:199:GLN:HB3	2.12	0.50
1:D:113:SER:N	3:D:294:HOH:O	2.15	0.50
1:A:167:LEU:C	1:A:167:LEU:HD12	2.32	0.49
1:C:99:GLY:HA3	1:C:233:MET:O	2.12	0.49
1:D:99:GLY:HA3	1:D:233:MET:O	2.12	0.49
1:A:199:GLN:O	1:A:199:GLN:CG	2.60	0.49
1:C:241:GLU:CD	3:C:316:HOH:O	2.51	0.49
1:D:195:GLN:OE1	3:D:766:HOH:O	2.17	0.49
1:A:70:ASN:ND2	1:A:93:ASN:HA	2.27	0.49
1:A:114:VAL:HG11	1:A:117:PHE:HB2	1.93	0.49
1:C:198:TYR:O	1:C:199:GLN:HB3	2.12	0.49
1:B:71:PRO:HA	1:B:152:LYS:HE3	1.94	0.49
1:A:104:TYR:CE2	1:A:108:ARG:HD2	2.48	0.49
1:A:146:GLY:N	3:A:566:HOH:O	1.90	0.49
1:B:137:GLY:HA3	1:B:156:TRP:HB3	1.95	0.49
1:C:104:TYR:CE2	1:C:108:ARG:HD2	2.48	0.49
1:A:78:THR:CG2	1:A:79:ALA:N	2.76	0.48
1:D:137:GLY:HA3	1:D:156:TRP:HB3	1.95	0.48
1:C:167:LEU:HD12	1:C:167:LEU:C	2.33	0.48
1:B:265:ARG:NH2	3:B:280:HOH:O	2.42	0.48
1:B:110:GLN:OE1	1:B:265:ARG:HD2	2.14	0.48
1:B:78:THR:CG2	1:B:79:ALA:N	2.76	0.48
1:D:198:TYR:O	1:D:199:GLN:HB3	2.14	0.48
1:D:84:TYR:HD2	3:D:644:HOH:O	1.89	0.48
1:B:198:TYR:O	1:B:199:GLN:HB3	2.14	0.47
1:B:214:LYS:CE	1:B:216:PHE:CE2	2.96	0.47
1:A:72:GLU:HG3	3:A:754:HOH:O	2.14	0.47
1:A:241:GLU:CD	3:A:320:HOH:O	2.53	0.47
1:C:78:THR:CG2	1:C:79:ALA:N	2.77	0.47
1:C:110:GLN:OE1	1:C:265:ARG:NH2	2.48	0.47
1:C:137:GLY:HA3	1:C:156:TRP:HB3	1.97	0.46
1:A:219:GLU:OE1	1:D:236:TYR:OH	2.33	0.46
1:A:166:LYS:O	1:B:89:PRO:HB2	2.16	0.46
1:B:113:SER:OG	1:B:266:ASN:HB2	2.15	0.46
1:C:110:GLN:HB3	1:C:265:ARG:HH21	1.81	0.46
3:A:422:HOH:O	1:B:88:THR:HG21	2.15	0.46
1:C:199:GLN:O	1:C:199:GLN:CG	2.64	0.45
1:A:137:GLY:HA3	1:A:156:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:SER:HB2	1:C:91:SER:H	1.58	0.45
1:A:132:HIS:HD2	3:A:16:HOH:O	1.99	0.45
1:C:88:THR:CG2	1:C:89:PRO:CD	2.95	0.45
1:A:174:ASP:OD2	3:A:592:HOH:O	2.20	0.44
1:B:84:TYR:HA	1:B:112:SER:O	2.18	0.44
1:C:88:THR:HG22	1:C:89:PRO:CD	2.46	0.44
1:A:74:GLU:HB2	1:A:76:LEU:HG	1.99	0.44
1:B:74:GLU:HB2	1:B:76:LEU:HG	1.99	0.44
1:D:74:GLU:HB2	1:D:76:LEU:HG	1.99	0.43
1:B:96:CYS:HB2	1:B:141:ALA:O	2.19	0.43
1:D:211:ARG:NH2	1:D:241:GLU:HG3	2.34	0.43
1:A:57:HIS:ND1	1:A:86:VAL:HG11	2.34	0.43
1:D:54:ALA:N	1:D:83:SER:HG	2.17	0.42
1:A:236:TYR:OH	1:D:219:GLU:OE1	2.36	0.42
1:B:92:ASP:O	1:B:93:ASN:HB2	2.20	0.42
1:C:198:TYR:O	1:C:199:GLN:CB	2.67	0.42
1:A:115:SER:HB3	1:A:266:ASN:OD1	2.19	0.42
1:C:219:GLU:CD	3:C:764:HOH:O	2.55	0.42
1:B:73:CYS:O	1:B:152:LYS:NZ	2.44	0.42
1:A:113:SER:OG	1:A:266:ASN:HB2	2.20	0.42
1:B:112:SER:HA	3:B:603:HOH:O	2.19	0.42
1:A:72:GLU:CB	1:A:93:ASN:ND2	2.83	0.41
1:D:214:LYS:HE2	3:D:417:HOH:O	2.18	0.41
1:C:113:SER:OG	1:C:266:ASN:HB2	2.20	0.41
1:A:96:CYS:HB2	1:A:141:ALA:O	2.21	0.41
1:C:115:SER:HB3	1:C:266:ASN:OD1	2.20	0.41
1:B:154:LEU:HB3	1:B:255:VAL:HG12	2.01	0.41
1:A:198:TYR:O	1:A:199:GLN:CB	2.67	0.41
1:D:80:SER:O	1:D:116:SER:HA	2.21	0.41
1:D:115:SER:HB3	1:D:266:ASN:OD1	2.20	0.41
1:A:54:ALA:HB1	1:A:55:PRO:HD2	2.03	0.41
1:A:74:GLU:C	1:A:76:LEU:N	2.74	0.41
1:A:154:LEU:HB3	1:A:255:VAL:HG12	2.03	0.41
1:C:154:LEU:HB3	1:C:255:VAL:HG12	2.04	0.41
1:C:96:CYS:HB2	1:C:141:ALA:O	2.21	0.40
1:B:54:ALA:N	1:B:83:SER:HG	2.19	0.40
1:C:72:GLU:HG3	1:C:93:ASN:OD1	2.21	0.40
1:A:199:GLN:HG3	3:A:598:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	212/214 (99%)	203 (96%)	8 (4%)	1 (0%)	29	18
1	B	213/214 (100%)	205 (96%)	8 (4%)	0	100	100
1	C	213/214 (100%)	204 (96%)	9 (4%)	0	100	100
1	D	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
All	All	851/856 (99%)	819 (96%)	31 (4%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ASN

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	186/186 (100%)	176 (95%)	10 (5%)	22	13
1	B	187/186 (100%)	180 (96%)	7 (4%)	34	25
1	C	187/186 (100%)	176 (94%)	11 (6%)	19	10
1	D	187/186 (100%)	176 (94%)	11 (6%)	19	10
All	All	747/744 (100%)	708 (95%)	39 (5%)	23	14

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	88	THR
1	A	107	LEU
1	A	152	LYS
1	A	157	LEU
1	A	167	LEU
1	A	211	ARG
1	A	219	GLU
1	A	225	LYS
1	A	258	ARG
1	B	78	THR
1	B	88	THR
1	B	107	LEU
1	B	114	VAL
1	B	167	LEU
1	B	219	GLU
1	B	258	ARG
1	C	78	THR
1	C	91	SER
1	C	92	ASP
1	C	101	PHE
1	C	114	VAL
1	C	152	LYS
1	C	167	LEU
1	C	177	LYS
1	C	211	ARG
1	C	219	GLU
1	C	265	ARG
1	D	60	LYS
1	D	78	THR
1	D	101	PHE
1	D	116	SER
1	D	152	LYS
1	D	162	ASN
1	D	167	LEU
1	D	211	ARG
1	D	214	LYS
1	D	219	GLU
1	D	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	132	HIS
1	A	162	ASN
1	A	194	GLN
1	A	199	GLN
1	A	253	ASN
1	B	93	ASN
1	B	132	HIS
1	B	162	ASN
1	B	194	GLN
1	B	199	GLN
1	B	253	ASN
1	C	132	HIS
1	C	144	HIS
1	C	162	ASN
1	C	194	GLN
1	C	199	GLN
1	C	253	ASN
1	D	110	GLN
1	D	132	HIS
1	D	162	ASN
1	D	194	GLN
1	D	195	GLN
1	D	199	GLN
1	D	253	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	#$|Z| > 2$
2	TAU	C	1	-	6,6,6	2.25	3 (50%)	6,8,8	2.78	3 (50%)
2	TAU	A	1	-	6,6,6	1.79	3 (50%)	6,8,8	3.02	4 (66%)

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
2	TAU	C	1	-	-	0/4/4/4	-
2	TAU	A	1	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	TAU	O3-S	-3.45	1.34	1.45
2	C	1	TAU	O2-S	-3.16	1.36	1.47
2	A	1	TAU	O1-S	-2.86	1.36	1.45
2	C	1	TAU	O1-S	-2.79	1.36	1.45
2	A	1	TAU	O2-S	-2.44	1.39	1.47
2	A	1	TAU	O3-S	-2.21	1.38	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	TAU	O1-S-C2	5.61	113.67	106.92
2	C	1	TAU	O1-S-C2	5.34	113.34	106.92
2	A	1	TAU	O3-S-C2	-2.99	103.32	106.92
2	A	1	TAU	O2-S-C2	2.81	110.31	105.77
2	C	1	TAU	O3-S-C2	2.61	110.06	106.92
2	A	1	TAU	O2-S-O3	-2.46	105.27	111.27
2	C	1	TAU	O2-S-O1	-2.37	105.48	111.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	TAU	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	214/214 (100%)	0.25	14 (6%)	18	21	12, 22, 62, 185	0
1	B	214/214 (100%)	0.21	11 (5%)	28	31	13, 23, 47, 170	0
1	C	214/214 (100%)	0.25	13 (6%)	21	24	11, 22, 64, 178	0
1	D	214/214 (100%)	0.20	11 (5%)	28	31	13, 22, 54, 144	0
All	All	856/856 (100%)	0.23	49 (5%)	23	26	11, 22, 57, 185	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	THR	20.6
1	B	267	ALA	15.6
1	C	77	SER	14.4
1	A	77	SER	11.3
1	C	75	SER	10.9
1	C	76	LEU	10.4
1	A	76	LEU	8.4
1	A	92	ASP	8.3
1	D	267	ALA	8.2
1	D	77	SER	7.9
1	B	76	LEU	7.8
1	C	267	ALA	7.6
1	A	75	SER	7.6
1	D	76	LEU	7.4
1	C	90	SER	7.3
1	C	78	THR	6.8
1	B	77	SER	6.8
1	D	75	SER	6.3
1	B	78	THR	6.3
1	B	146	GLY	6.0
1	D	78	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	75	SER	5.4
1	C	74	GLU	4.3
1	A	74	GLU	4.1
1	C	79	ALA	3.8
1	D	145	ALA	3.8
1	B	74	GLU	3.6
1	D	74	GLU	3.6
1	C	266	ASN	3.5
1	A	93	ASN	3.2
1	C	89	PRO	3.1
1	B	145	ALA	3.1
1	A	267	ALA	3.1
1	D	266	ASN	3.0
1	A	91	SER	2.9
1	D	146	GLY	2.8
1	C	93	ASN	2.8
1	B	266	ASN	2.8
1	A	57	HIS	2.8
1	A	79	ALA	2.7
1	A	89	PRO	2.7
1	D	73	CYS	2.6
1	A	266	ASN	2.5
1	A	146	GLY	2.4
1	B	84	TYR	2.3
1	C	113	SER	2.2
1	D	84	TYR	2.2
1	B	79	ALA	2.1
1	C	265	ARG	2.0

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	TAU	A	1	7/7	0.93	0.16	36,36,36,36	0
2	TAU	C	1	7/7	0.93	0.20	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK