Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 03:09 PM EDT

PDB ID	:	3BD0
Title	:	Crystal structure of Memo, form II
Authors	:	Qiu, C.
Deposited on	:	2007-11-13
Resolution	:	3.01 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.35
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)	:	2.35
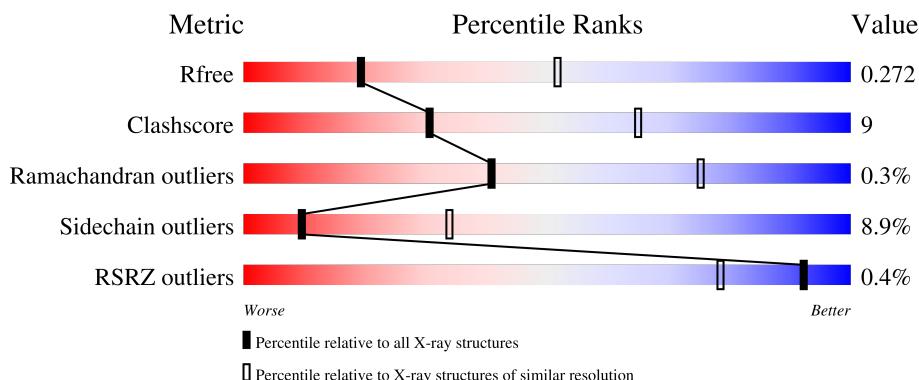
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
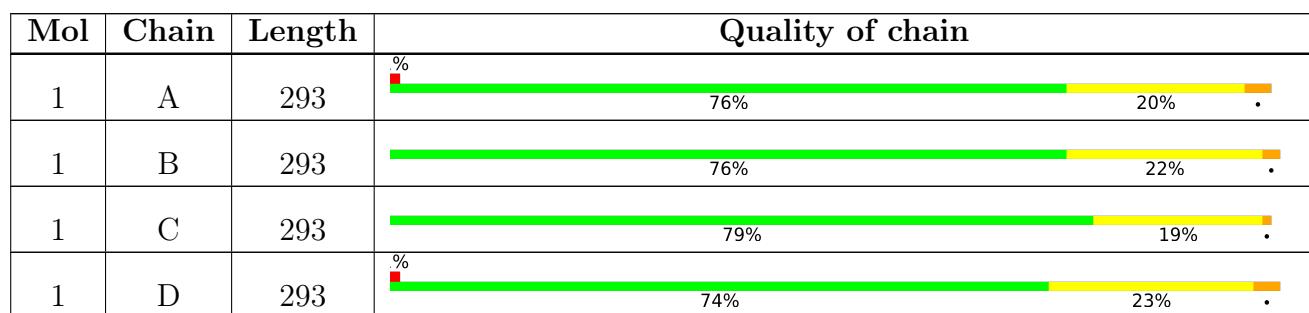
The reported resolution of this entry is 3.01 Å.

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		0.272
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		8.9%
RSRZ outliers		0.4%

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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	293	76% 20%
1	B	293	76% 22%
1	C	293	79% 19%
1	D	293	74% 23%

2 Entry composition ⓘ
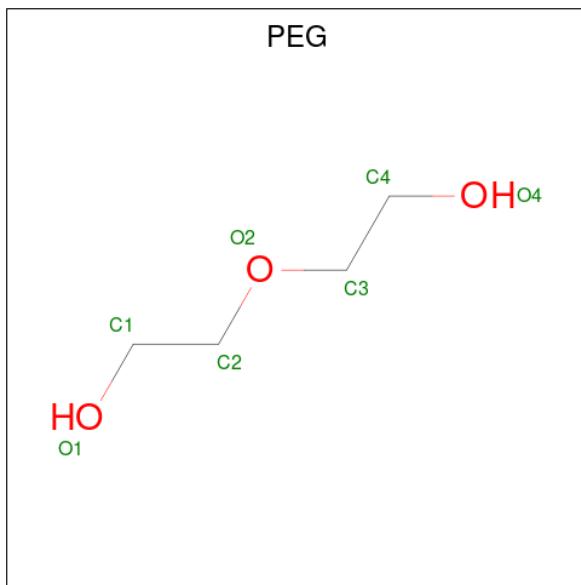
There are 3 unique types of molecules in this entry. The entry contains 9426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein MEMO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2339	1482	403	439	15			
1	B	293	Total	C	N	O	S	0	0	0
			2339	1482	403	439	15			
1	C	293	Total	C	N	O	S	0	0	0
			2339	1482	403	439	15			
1	D	293	Total	C	N	O	S	0	0	0
			2339	1482	403	439	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
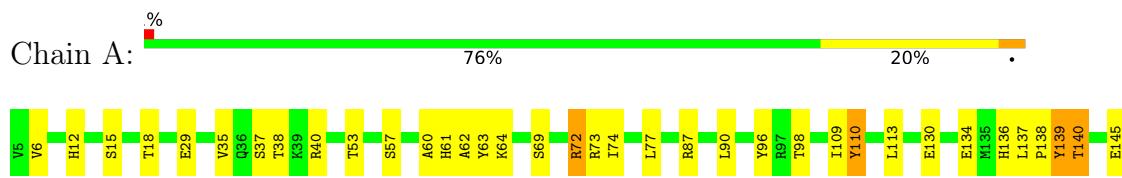
- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total 13	O 13	0	0
3	B	13	Total 13	O 13	0	0
3	C	17	Total 17	O 17	0	0
3	D	20	Total 20	O 20	0	0
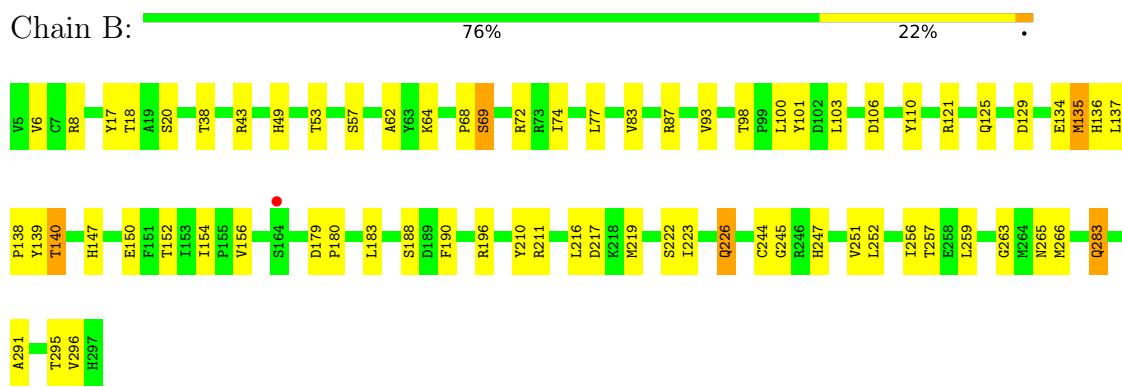
3 Residue-property plots ⓘ

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.
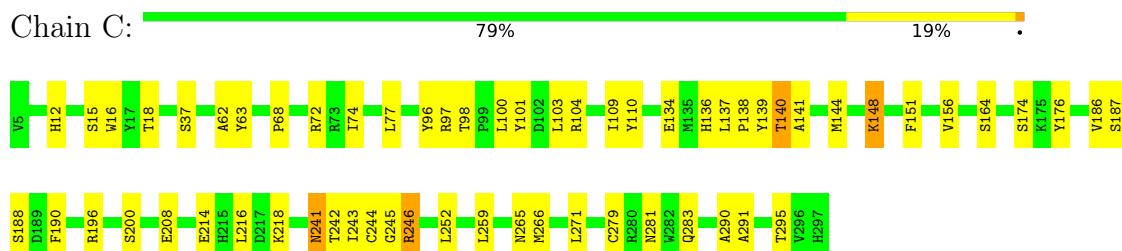
- Molecule 1: Protein MEMO1
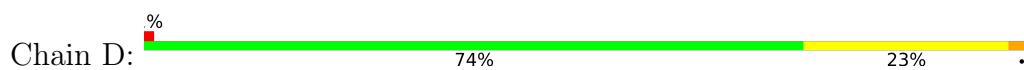
Chain A:

- Molecule 1: Protein MEMO1

Chain B:

- Molecule 1: Protein MEMO1

Chain C:

- Molecule 1: Protein MEMO1

Chain D:

V5 R8 S11 H12 W16 E29 Q36 S37 T38 K39 A44 A47 P48 H49 T53 Y54 S57 A60 Y63 K64 D67 P68 S69 R72 R73 R87 S91 S92 V93 Y96 R97 T98 P99 L100 Y101 D106 Q107 K108 I109 Y110 E128

E134 M135 H136 L137 P138 Y139 T140 E150 F151 T152 I153 I154 P155 S164 K175 A178 S181 V186 S187 S188 H192 R196 F197 S200 D203 L216 D217 M221 S222 Q226 N241 T242 I243 C244 G245 L252 I256 L259 N265 M266 S267 F268

S269 F270 L271 N272 Y273 N281 W282 Q283 L294 T295 V296 H297
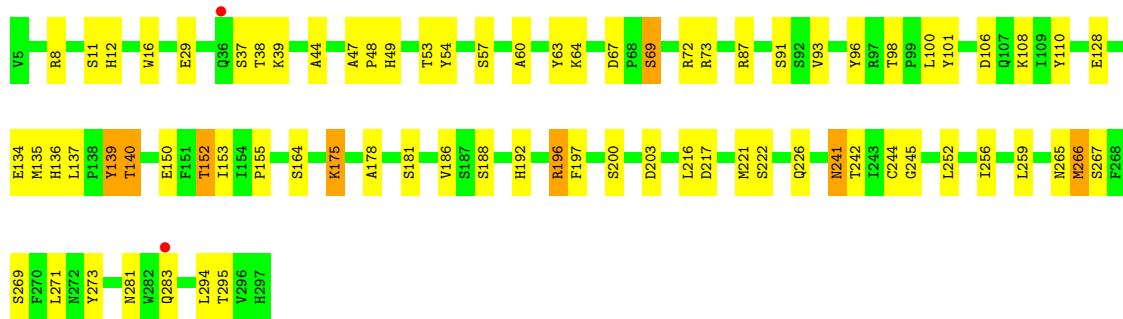
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.88Å 88.31Å 97.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 3.01 29.68 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.68-3.01) 99.6 (29.68-3.01)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.280 0.209 , 0.272	Depositor DCC
R_{free} test set	1249 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.833	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 29.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9426	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 46.18 % 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 1.1878e-04. 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: PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.54	0/2401	0.64	1/3252 (0.0%)
1	B	0.53	0/2401	0.68	0/3252
1	C	0.54	1/2401 (0.0%)	0.68	0/3252
1	D	0.53	0/2401	0.67	0/3252
All	All	0.53	1/9604 (0.0%)	0.67	1/13008 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	CYS	CB-SG	-5.14	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	LEU	CA-CB-CG	5.04	126.90	115.30

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	2339	0	2255	43	0
1	B	2339	0	2255	44	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2339	0	2255	35	0
1	D	2339	0	2255	50	0
2	A	7	0	10	1	0
3	A	13	0	0	0	0
3	B	13	0	0	1	0
3	C	17	0	0	1	0
3	D	20	0	0	0	0
All	All	9426	0	9030	169	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 9.

All (169) 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:B:98:THR:HG22	1:B:100:LEU:H	1.28	0.99
1:D:16:TRP:HB2	1:D:135:MET:HE1	1.47	0.97
1:D:16:TRP:CB	1:D:135:MET:HE1	1.95	0.95
1:C:68:PRO:HA	1:C:144:MET:CE	1.96	0.94
1:D:98:THR:HG22	1:D:100:LEU:H	1.34	0.90
1:C:68:PRO:HA	1:C:144:MET:HE1	1.59	0.83
1:A:72:ARG:CG	1:A:72:ARG:HH11	1.91	0.82
1:D:16:TRP:CB	1:D:135:MET:CE	2.59	0.81
1:A:137:LEU:HB2	1:A:138:PRO:HD3	1.62	0.80
1:C:68:PRO:HA	1:C:144:MET:HE3	1.63	0.79
1:B:211:ARG:HD2	3:B:309:HOH:O	1.87	0.74
1:D:16:TRP:HB3	1:D:135:MET:CE	2.18	0.73
1:A:77:LEU:HD22	1:A:156:VAL:HB	1.69	0.73
1:D:73:ARG:HH21	1:D:181:SER:HB2	1.54	0.72
1:A:219:MET:HG3	1:B:263:GLY:HA3	1.71	0.71
1:D:16:TRP:HB3	1:D:135:MET:HE1	1.70	0.69
1:C:98:THR:HG22	1:C:100:LEU:H	1.55	0.69
1:D:96:TYR:HD2	1:D:137:LEU:HD11	1.59	0.67
1:B:98:THR:HB	1:B:101:TYR:O	1.94	0.67
1:A:188:SER:HB2	1:A:245:GLY:HA3	1.77	0.66
1:B:49:HIS:CE1	1:B:244:CYS:SG	2.88	0.66
1:B:98:THR:HG22	1:B:100:LEU:N	2.05	0.66
1:D:98:THR:HB	1:D:101:TYR:O	1.96	0.65
1:A:72:ARG:HH11	1:A:72:ARG:HG3	1.60	0.65
1:C:188:SER:HB2	1:C:245:GLY:HA3	1.79	0.64
1:C:12:HIS:HD2	1:C:134:GLU:OE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HB2	1:A:147:HIS:HD2	1.63	0.64
1:B:69:SER:HA	1:B:147:HIS:CE1	2.33	0.63
1:B:74:ILE:HG12	1:B:183:LEU:HD23	1.80	0.62
1:B:137:LEU:HB2	1:B:138:PRO:HD3	1.80	0.62
1:A:146:SER:HB2	1:A:147:HIS:CD2	2.34	0.62
1:C:98:THR:HB	1:C:101:TYR:O	1.99	0.62
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.14	0.61
1:C:259:LEU:HB2	1:C:266:MET:CE	2.31	0.61
1:A:63:TYR:HE1	1:A:140:THR:HG23	1.65	0.60
1:D:252:LEU:O	1:D:256:ILE:HG13	2.02	0.60
1:C:241:ASN:HD22	1:C:242:THR:H	1.51	0.59
1:D:39:LYS:HE2	1:D:269:SER:OG	2.02	0.59
1:D:217:ASP:HB3	1:D:221:MET:CE	2.32	0.59
1:B:17:TYR:CD1	1:B:135:MET:CE	2.87	0.58
1:B:49:HIS:HE1	1:B:244:CYS:SG	2.27	0.57
1:C:74:ILE:HG21	1:C:140:THR:HG21	1.85	0.57
1:B:77:LEU:HD22	1:B:156:VAL:HB	1.86	0.57
1:C:98:THR:HG22	1:C:100:LEU:N	2.21	0.56
1:A:60:ALA:HB2	1:A:139:TYR:OH	2.06	0.56
1:D:106:ASP:HB2	1:D:152:THR:HB	1.87	0.56
1:A:12:HIS:HD2	1:A:134:GLU:OE1	1.88	0.55
1:B:188:SER:HB2	1:B:245:GLY:HA3	1.89	0.55
1:C:186:VAL:HG21	1:C:252:LEU:HD22	1.88	0.55
1:A:241:ASN:HD22	1:A:242:THR:H	1.55	0.54
1:D:217:ASP:HB3	1:D:221:MET:HE3	1.89	0.54
1:B:259:LEU:CD1	1:B:266:MET:HE1	2.38	0.54
1:C:259:LEU:HB2	1:C:266:MET:HE3	1.88	0.54
1:B:219:MET:O	1:B:223:ILE:HD12	2.08	0.54
1:D:241:ASN:HD22	1:D:242:THR:H	1.56	0.53
1:B:69:SER:HA	1:B:147:HIS:HE1	1.73	0.53
1:A:137:LEU:N	1:A:138:PRO:CD	2.72	0.52
1:B:74:ILE:HG21	1:B:140:THR:HG21	1.92	0.52
1:D:188:SER:HB2	1:D:245:GLY:HA3	1.91	0.52
1:D:67:ASP:OD1	1:D:69:SER:HB2	2.09	0.52
1:A:219:MET:HE1	1:A:239:TYR:CE2	2.45	0.51
1:D:44:ALA:HB3	1:D:294:LEU:HB3	1.93	0.51
1:D:221:MET:HE1	1:D:273:TYR:CD2	2.45	0.51
1:C:109:ILE:HG12	1:C:176:TYR:CE2	2.46	0.51
1:C:96:TYR:HD2	1:C:137:LEU:HD11	1.76	0.51
1:A:74:ILE:HG12	1:A:183:LEU:HD23	1.92	0.51
1:C:137:LEU:HB2	1:C:138:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HH11	1:A:72:ARG:HG2	1.68	0.51
1:D:16:TRP:HB2	1:D:135:MET:CE	2.25	0.51
1:D:98:THR:HG22	1:D:100:LEU:N	2.14	0.51
1:D:222:SER:O	1:D:226:GLN:HG2	2.11	0.51
1:A:96:TYR:HD2	1:A:137:LEU:HD11	1.75	0.51
1:C:12:HIS:CD2	1:C:134:GLU:OE1	2.61	0.50
1:B:17:TYR:HD1	1:B:135:MET:CE	2.25	0.50
1:B:210:TYR:CE1	1:B:211:ARG:HG3	2.47	0.50
1:B:223:ILE:HA	1:B:226:GLN:HG3	1.92	0.50
1:C:136:HIS:HE1	1:C:187:SER:CB	2.24	0.50
1:B:18:THR:HG22	1:B:20:SER:H	1.77	0.50
1:A:90:LEU:HB3	1:A:110:TYR:CZ	2.47	0.49
1:A:222:SER:O	1:A:226:GLN:HG2	2.11	0.49
1:B:106:ASP:HB3	1:B:154:ILE:CD1	2.42	0.49
1:D:91:SER:OG	1:D:93:VAL:HG22	2.13	0.49
1:A:226:GLN:HA	1:B:180:PRO:HG3	1.94	0.49
1:A:296:VAL:HG12	1:A:297:HIS:N	2.27	0.49
1:B:266:MET:HG2	1:B:296:VAL:HG22	1.93	0.49
1:B:62:ALA:HB2	1:B:291:ALA:HB1	1.94	0.49
1:D:186:VAL:HG21	1:D:252:LEU:HD22	1.95	0.49
1:C:63:TYR:HE1	1:C:140:THR:HG23	1.78	0.48
1:B:259:LEU:HD12	1:B:266:MET:HE1	1.95	0.48
1:D:64:LYS:O	1:D:64:LYS:HG3	2.13	0.48
1:D:8:ARG:HB2	1:D:93:VAL:HG21	1.96	0.47
1:D:16:TRP:CB	1:D:135:MET:HE3	2.43	0.47
1:B:150:GLU:HG3	1:D:108:LYS:HD2	1.96	0.47
1:A:63:TYR:CE1	1:A:140:THR:HG23	2.49	0.47
1:B:8:ARG:HB2	1:B:93:VAL:HG21	1.97	0.47
1:B:136:HIS:O	1:B:140:THR:OG1	2.31	0.47
1:D:178:ALA:HB2	1:D:259:LEU:HD21	1.96	0.47
1:A:245:GLY:O	1:A:249:ILE:HG13	2.15	0.46
1:C:77:LEU:HD22	1:C:156:VAL:HB	1.97	0.46
1:C:214:GLU:OE2	1:C:218:LYS:NZ	2.48	0.46
1:A:73:ARG:HD2	1:A:109:ILE:CD1	2.45	0.46
1:A:238:LYS:HD3	1:A:239:TYR:CE2	2.51	0.46
1:D:134:GLU:O	1:D:137:LEU:HB2	2.16	0.46
1:A:241:ASN:HD22	1:A:242:THR:N	2.13	0.46
1:D:153:ILE:HD12	1:D:155:PRO:HG3	1.98	0.46
1:B:106:ASP:HB2	1:B:152:THR:HB	1.97	0.46
1:C:103:LEU:HD11	1:C:141:ALA:HB2	1.98	0.46
1:C:136:HIS:O	1:C:140:THR:OG1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ASP:OD1	1:D:203:ASP:C	2.54	0.46
1:D:259:LEU:HB3	1:D:266:MET:HE1	1.97	0.46
1:C:15:SER:OG	1:C:16:TRP:HD1	1.99	0.46
1:D:217:ASP:O	1:D:221:MET:HG3	2.16	0.46
1:C:136:HIS:CE1	1:C:187:SER:HB2	2.51	0.46
1:D:241:ASN:HD22	1:D:242:THR:N	2.14	0.46
1:C:136:HIS:CE1	1:C:187:SER:CB	3.00	0.45
1:D:12:HIS:HD2	1:D:134:GLU:OE1	1.99	0.45
1:C:190:PHE:CE1	1:C:290:ALA:HB3	2.51	0.45
1:D:136:HIS:O	1:D:140:THR:OG1	2.29	0.45
1:D:60:ALA:HB2	1:D:139:TYR:OH	2.16	0.45
1:D:192:HIS:HD2	1:D:242:THR:O	2.00	0.45
1:A:35:VAL:HG11	1:A:61:HIS:HA	1.99	0.44
1:A:296:VAL:CG1	1:A:297:HIS:N	2.80	0.44
1:A:136:HIS:O	1:A:140:THR:OG1	2.29	0.44
1:A:219:MET:CE	1:A:239:TYR:CE2	3.01	0.44
1:C:241:ASN:HD22	1:C:242:THR:N	2.13	0.44
1:C:243:ILE:O	1:C:246:ARG:HG2	2.18	0.44
1:D:221:MET:CE	1:D:273:TYR:CD2	3.00	0.44
1:B:103:LEU:HD12	1:B:137:LEU:HD22	2.00	0.44
1:B:179:ASP:OD1	1:B:180:PRO:HD2	2.17	0.43
1:D:11:SER:OG	1:D:128:GLU:O	2.28	0.43
1:D:72:ARG:HD2	1:D:150:GLU:O	2.17	0.43
1:B:125:GLN:O	1:B:129:ASP:HB2	2.18	0.43
1:A:15:SER:HB2	2:A:298:PEG:H21	2.00	0.43
1:D:196:ARG:HD2	1:D:197:PHE:CE1	2.53	0.43
1:B:252:LEU:HG	1:B:256:ILE:CD1	2.48	0.43
1:A:62:ALA:HB2	1:A:291:ALA:HB1	2.00	0.43
1:B:17:TYR:CD1	1:B:135:MET:HE1	2.53	0.43
1:B:43:ARG:O	1:B:183:LEU:HA	2.19	0.43
1:B:68:PRO:O	1:B:72:ARG:NH1	2.52	0.43
1:A:130:GLU:HG2	1:A:157:LEU:CD1	2.49	0.43
1:A:137:LEU:N	1:A:138:PRO:HD2	2.33	0.43
1:A:40:ARG:HH21	1:A:64:LYS:HD2	1.85	0.42
1:C:259:LEU:HB2	1:C:266:MET:HE1	2.01	0.42
1:B:17:TYR:HD1	1:B:135:MET:HE1	1.83	0.42
1:C:101:TYR:CG	1:C:148:LYS:HE3	2.54	0.42
1:D:259:LEU:HB2	1:D:266:MET:HE3	2.01	0.42
1:D:49:HIS:CE1	1:D:244:CYS:SG	3.13	0.42
1:A:137:LEU:H	1:A:138:PRO:HD2	1.84	0.42
1:D:96:TYR:CD2	1:D:137:LEU:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TYR:CZ	1:C:148:LYS:HG3	2.54	0.42
1:D:63:TYR:HE1	1:D:140:THR:HG23	1.85	0.42
1:B:17:TYR:OH	1:B:134:GLU:OE2	2.29	0.42
1:B:252:LEU:HG	1:B:256:ILE:HD12	2.01	0.42
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.80	0.41
1:B:247:HIS:O	1:B:251:VAL:HG23	2.20	0.41
1:B:64:LYS:O	1:B:64:LYS:HG3	2.19	0.41
1:A:63:TYR:OH	1:A:136:HIS:HB3	2.20	0.41
1:A:259:LEU:HB2	1:A:266:MET:CE	2.50	0.41
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.68	0.41
1:C:62:ALA:HB2	1:C:291:ALA:HB1	2.01	0.41
1:A:196:ARG:HD2	1:A:197:PHE:CZ	2.56	0.41
1:C:72:ARG:O	1:C:151:PHE:HA	2.21	0.41
1:D:221:MET:HE1	1:D:273:TYR:HD2	1.86	0.41
1:A:191:CYS:HB2	1:A:241:ASN:HD21	1.86	0.40
1:B:283:GLN:HE21	1:B:283:GLN:N	2.19	0.40
1:C:97:ARG:HB3	3:C:299:HOH:O	2.22	0.40
1:B:190:PHE:HB3	1:B:217:ASP:OD1	2.22	0.40
1:D:175:LYS:HB2	1:D:175:LYS:HE2	1.69	0.40
1:D:47:ALA:HB1	1:D:48:PRO:HD2	2.03	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	291/293 (99%)	277 (95%)	12 (4%)	2 (1%)	22	59
1	B	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
1	C	291/293 (99%)	280 (96%)	10 (3%)	1 (0%)	41	75
1	D	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
All	All	1164/1172 (99%)	1116 (96%)	45 (4%)	3 (0%)	41	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	148	LYS
1	C	148	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	255/255 (100%)	229 (90%)	26 (10%)	7	27
1	B	255/255 (100%)	235 (92%)	20 (8%)	12	40
1	C	255/255 (100%)	235 (92%)	20 (8%)	12	40
1	D	255/255 (100%)	230 (90%)	25 (10%)	8	29
All	All	1020/1020 (100%)	929 (91%)	91 (9%)	9	34

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	18	THR
1	A	29	GLU
1	A	37	SER
1	A	38	THR
1	A	53	THR
1	A	57	SER
1	A	69	SER
1	A	72	ARG
1	A	87	ARG
1	A	98	THR
1	A	110	TYR
1	A	139	TYR
1	A	140	THR
1	A	146	SER
1	A	154	ILE
1	A	196	ARG

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Mol	Chain	Res	Type
1	A	200	SER
1	A	208	GLU
1	A	216	LEU
1	A	222	SER
1	A	241	ASN
1	A	244	CYS
1	A	271	LEU
1	A	276	SER
1	A	281	ASN
1	B	6	VAL
1	B	38	THR
1	B	53	THR
1	B	57	SER
1	B	69	SER
1	B	83	VAL
1	B	87	ARG
1	B	110	TYR
1	B	121	ARG
1	B	135	MET
1	B	139	TYR
1	B	140	THR
1	B	196	ARG
1	B	216	LEU
1	B	222	SER
1	B	226	GLN
1	B	257	THR
1	B	265	ASN
1	B	283	GLN
1	B	295	THR
1	C	18	THR
1	C	37	SER
1	C	104	ARG
1	C	110	TYR
1	C	139	TYR
1	C	140	THR
1	C	164	SER
1	C	174	SER
1	C	196	ARG
1	C	200	SER
1	C	208	GLU
1	C	216	LEU
1	C	241	ASN

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Mol	Chain	Res	Type
1	C	244	CYS
1	C	246	ARG
1	C	265	ASN
1	C	271	LEU
1	C	281	ASN
1	C	283	GLN
1	C	295	THR
1	D	29	GLU
1	D	37	SER
1	D	38	THR
1	D	53	THR
1	D	54	TYR
1	D	57	SER
1	D	69	SER
1	D	87	ARG
1	D	110	TYR
1	D	139	TYR
1	D	140	THR
1	D	152	THR
1	D	164	SER
1	D	175	LYS
1	D	196	ARG
1	D	200	SER
1	D	216	LEU
1	D	241	ASN
1	D	265	ASN
1	D	266	MET
1	D	267	SER
1	D	271	LEU
1	D	281	ASN
1	D	283	GLN
1	D	295	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	25	ASN
1	A	49	HIS
1	A	147	HIS
1	A	167	GLN
1	A	192	HIS

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Mol	Chain	Res	Type
1	A	234	ASN
1	A	240	HIS
1	A	241	ASN
1	A	254	ASN
1	A	275	GLN
1	B	49	HIS
1	B	61	HIS
1	B	167	GLN
1	B	192	HIS
1	B	275	GLN
1	B	283	GLN
1	B	297	HIS
1	C	12	HIS
1	C	61	HIS
1	C	136	HIS
1	C	167	GLN
1	C	192	HIS
1	C	234	ASN
1	C	241	ASN
1	C	265	ASN
1	C	275	GLN
1	C	283	GLN
1	D	12	HIS
1	D	49	HIS
1	D	61	HIS
1	D	131	HIS
1	D	167	GLN
1	D	192	HIS
1	D	241	ASN
1	D	265	ASN
1	D	283	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	PEG	A	298	-	6,6,6	0.62	0	5,5,5	0.36	0

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	PEG	A	298	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	298	PEG	O1-C1-C2-O2
2	A	298	PEG	C1-C2-O2-C3
2	A	298	PEG	O2-C3-C4-O4
2	A	298	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	298	PEG	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(Å^2)	Q<0.9
1	A	293/293 (100%)	-0.35	2 (0%)	87	68	10, 19, 30, 35	1 (0%)
1	B	293/293 (100%)	-0.30	1 (0%)	94	83	11, 19, 30, 35	0
1	C	293/293 (100%)	-0.34	0	100	100	10, 19, 30, 35	0
1	D	293/293 (100%)	-0.35	2 (0%)	87	68	10, 18, 30, 35	0
All	All	1172/1172 (100%)	-0.33	5 (0%)	92	78	10, 19, 30, 35	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	GLN	2.5
1	D	283	GLN	2.5
1	A	283	GLN	2.3
1	A	281	ASN	2.2
1	B	164	SER	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	PEG	A	298	7/7	0.84	0.21	44,46,48,48	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