



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 4AUO / pdb_00004auo
Title : Crystal structure of MMP-1(E200A) in complex with a triple-helical collagen peptide
Authors : Manka, S.W.; Carafoli, F.; Visse, R.; Bihan, D.; Raynal, N.; Farndale, R.W.; Murphy, G.; Enghild, J.J.; Hohenester, E.; Nagase, H.
Deposited on : 2012-05-18
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

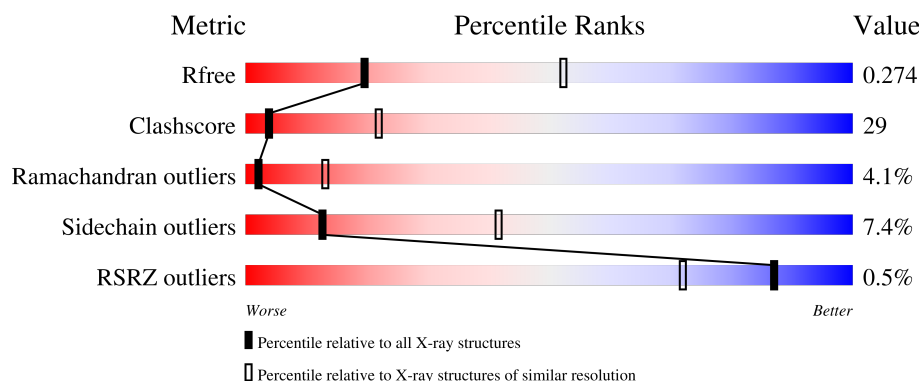
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	367	% 55% 38% 7%
1	B	367	56% 38% 5%
2	C	40	5% 40% 50% 8%
2	D	40	48% 32% 10% 10%
2	E	40	35% 38% 10% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	40	
2	G	40	
2	H	40	

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
2	HYP	D	965	-	-	X	-
2	HYP	E	965	-	-	X	-
2	HYP	H	971	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7387 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 INTERSTITIAL COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2986	1922	511	544	9			
1	B	367	Total	C	N	O	S	0	0	0
			2985	1921	510	545	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	ALA	GLU	engineered mutation	UNP P03956
B	200	ALA	GLU	engineered mutation	UNP P03956

- Molecule 2 is a protein called TRIPLE-HELICAL COLLAGEN PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	39	Total	C	N	O	0	0	0
			258	158	51	49			
2	D	36	Total	C	N	O	0	0	0
			243	148	48	47			
2	E	33	Total	C	N	O	0	0	0
			210	129	41	40			
2	F	36	Total	C	N	O	0	0	0
			239	146	48	45			
2	G	36	Total	C	N	O	0	0	0
			237	145	45	47			
2	H	33	Total	C	N	O	0	0	0
			210	129	41	40			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	Ca 4	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Zn 2	0	0
4	B	2	Total 2	Zn 2	0	0

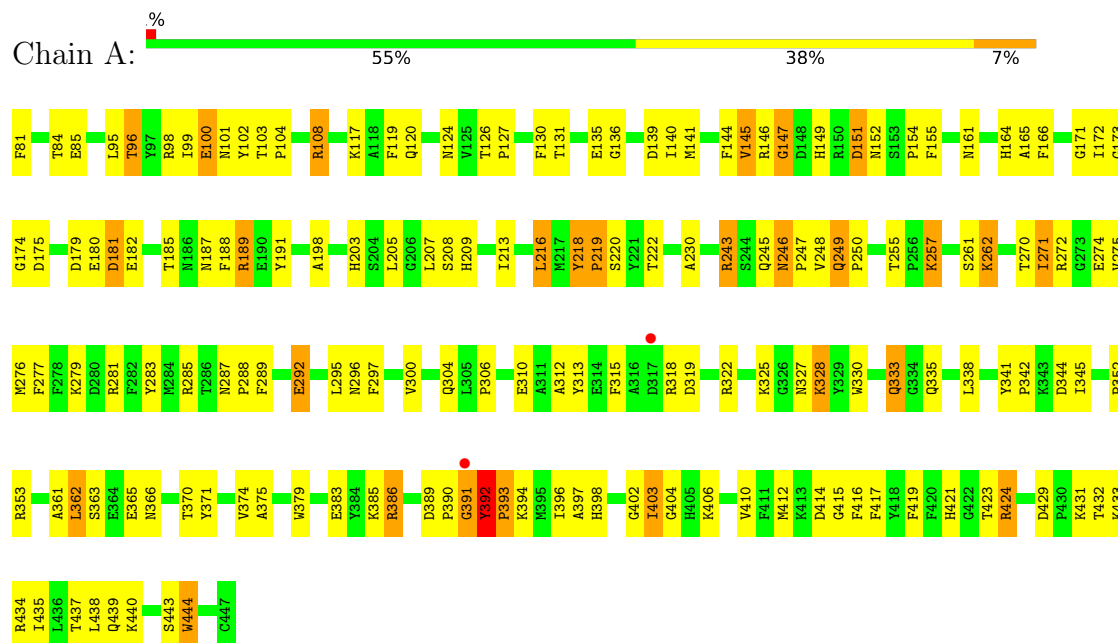
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	O 4	0	0
5	B	3	Total 3	O 3	0	0

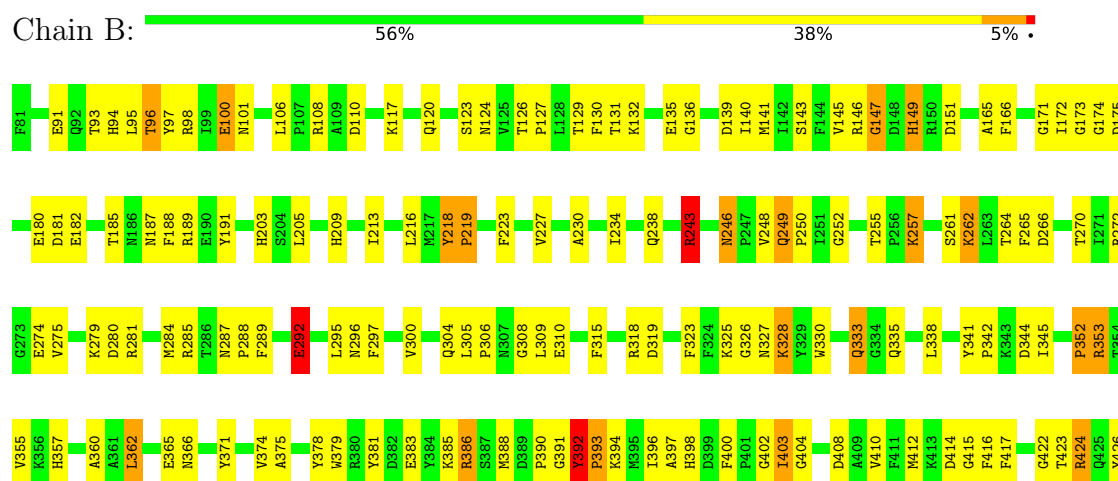
3 Residue-property plots

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: INTERSTITIAL COLLAGENASE

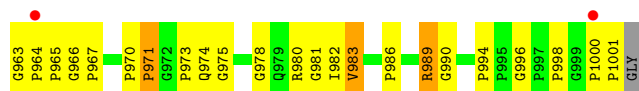


• Molecule 1: INTERSTITIAL COLLAGENASE

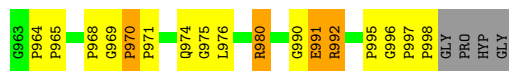




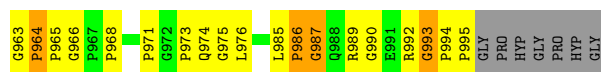
• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



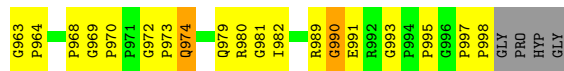
• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



• Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.67Å 102.24Å 80.73Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-3.00) 86.2 (20.00-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.98Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.211 , 0.273 0.212 , 0.274	Depositor DCC
R_{free} test set	2069 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.64% 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, CA, HYP

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	0.51	0/3086	0.98	11/4188 (0.3%)
1	B	0.51	0/3085	0.99	19/4187 (0.5%)
2	C	0.47	0/202	0.97	0/263
2	D	0.42	0/195	0.84	0/254
2	E	0.44	0/170	0.80	0/223
2	F	0.46	0/191	1.09	2/249 (0.8%)
2	G	0.46	0/189	0.92	0/247
2	H	0.45	0/170	0.96	0/223
All	All	0.50	0/7288	0.98	32/9834 (0.3%)

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ASP	CB-CA-C	-6.66	108.91	116.63
1	A	216	LEU	N-CA-C	-6.44	104.35	111.82
1	B	216	LEU	N-CA-C	-6.36	104.22	112.23
2	F	979	GLN	N-CA-C	-6.34	101.72	110.35
1	A	218	TYR	CA-C-N	6.19	127.57	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2986	0	2803	173	0
1	B	2985	0	2799	152	0
2	C	258	0	248	27	0
2	D	243	0	235	19	0
2	E	210	0	196	32	0
2	F	239	0	231	22	0
2	G	237	0	224	21	0
2	H	210	0	197	17	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
All	All	7387	0	6933	408	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 29.

The worst 5 of 408 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:403:ILE:HD12	1:B:404:GLY:H	1.15	1.07
1:A:403:ILE:HD12	1:A:404:GLY:H	1.23	1.01
1:B:386:ARG:HB3	1:B:386:ARG:HH11	1.32	0.94
1:B:333:GLN:HB2	1:B:338:LEU:HD21	1.48	0.94
1:B:403:ILE:HD12	1:B:404:GLY:N	1.82	0.93

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	365/367 (100%)	318 (87%)	31 (8%)	16 (4%)	2	12
1	B	365/367 (100%)	316 (87%)	37 (10%)	12 (3%)	3	17
2	C	31/40 (78%)	28 (90%)	2 (6%)	1 (3%)	3	18
2	D	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	5
2	E	26/40 (65%)	20 (77%)	3 (12%)	3 (12%)	0	1
2	F	29/40 (72%)	25 (86%)	3 (10%)	1 (3%)	3	17
2	G	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	5
2	H	27/40 (68%)	22 (82%)	5 (18%)	0	100	100
All	All	901/974 (92%)	775 (86%)	89 (10%)	37 (4%)	2	13

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
1	B	403	ILE
2	G	969	GLY
1	A	147	GLY
1	A	189	ARG

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	311/313 (99%)	290 (93%)	21 (7%)	14	45
1	B	311/313 (99%)	288 (93%)	23 (7%)	13	42
2	C	17/18 (94%)	16 (94%)	1 (6%)	18	50
2	D	17/18 (94%)	14 (82%)	3 (18%)	2	10
2	E	13/18 (72%)	13 (100%)	0	100	100
2	F	16/18 (89%)	13 (81%)	3 (19%)	1	9
2	G	16/18 (89%)	15 (94%)	1 (6%)	16	48
2	H	13/18 (72%)	12 (92%)	1 (8%)	12	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	714/734 (97%)	661 (93%)	53 (7%)	13	42

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	262	LYS
1	B	344	ASP
2	F	982	ILE
1	B	274	GLU
1	B	292	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	GLN
2	G	979	GLN
2	G	988	GLN
2	G	974	GLN
1	A	425	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

35 non-standard protein/DNA/RNA residues 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	HYP	C	965	2	7,8,9	0.51	0	5,10,12	1.14	0
2	HYP	E	968	2	7,8,9	0.59	0	5,10,12	1.35	0
2	HYP	F	971	2	7,8,9	0.63	0	5,10,12	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HYP	G	971	2	7,8,9	0.57	0	5,10,12	1.05	0
2	HYP	C	998	2	7,8,9	0.52	0	5,10,12	1.07	0
2	HYP	G	998	2	7,8,9	0.50	0	5,10,12	1.22	1 (20%)
2	HYP	F	965	2	7,8,9	0.55	0	5,10,12	1.21	1 (20%)
2	HYP	H	995	2	7,8,9	0.61	0	5,10,12	1.00	0
2	HYP	C	986	2	7,8,9	0.59	0	5,10,12	1.27	1 (20%)
2	HYP	D	971	2	7,8,9	0.59	0	5,10,12	1.20	1 (20%)
2	HYP	D	965	2	7,8,9	0.50	0	5,10,12	1.08	0
2	HYP	G	986	2	7,8,9	0.65	0	5,10,12	0.90	0
2	HYP	C	995	2	7,8,9	0.65	0	5,10,12	1.14	0
2	HYP	E	971	2	7,8,9	0.55	0	5,10,12	1.01	0
2	HYP	F	986	2	7,8,9	0.69	0	5,10,12	1.71	1 (20%)
2	HYP	C	1001	2	7,8,9	0.50	0	5,10,12	1.11	0
2	HYP	D	998	2	7,8,9	0.52	0	5,10,12	1.19	0
2	HYP	G	968	2	7,8,9	0.56	0	5,10,12	1.12	0
2	HYP	G	995	2	7,8,9	0.58	0	5,10,12	0.89	0
2	HYP	F	968	2	7,8,9	0.68	0	5,10,12	1.41	1 (20%)
2	HYP	E	965	2	7,8,9	0.49	0	5,10,12	1.13	0
2	HYP	D	986	2	7,8,9	0.59	0	5,10,12	0.93	0
2	HYP	D	968	2	7,8,9	0.57	0	5,10,12	1.23	1 (20%)
2	HYP	G	965	2	7,8,9	0.65	0	5,10,12	1.26	0
2	HYP	F	995	2	7,8,9	0.57	0	5,10,12	0.94	0
2	HYP	D	995	2	7,8,9	0.62	0	5,10,12	1.34	1 (20%)
2	HYP	H	986	2	7,8,9	0.66	0	5,10,12	1.68	1 (20%)
2	HYP	F	998	2	7,8,9	0.51	0	5,10,12	1.02	0
2	HYP	C	971	2	7,8,9	0.58	0	5,10,12	1.63	2 (40%)
2	HYP	H	971	2	7,8,9	0.74	0	5,10,12	1.31	1 (20%)
2	HYP	E	995	2	7,8,9	0.49	0	5,10,12	1.10	1 (20%)
2	HYP	E	986	2	7,8,9	0.57	0	5,10,12	1.54	1 (20%)
2	HYP	H	965	2	7,8,9	0.49	0	5,10,12	1.00	0
2	HYP	H	968	2	7,8,9	0.66	0	5,10,12	1.47	1 (20%)
2	HYP	C	968	2	7,8,9	0.54	0	5,10,12	1.05	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	HYP	C	965	2	-	0/0/11/13	0/1/1/1
2	HYP	E	968	2	-	0/0/11/13	0/1/1/1
2	HYP	F	971	2	-	0/0/11/13	0/1/1/1
2	HYP	G	971	2	-	0/0/11/13	0/1/1/1
2	HYP	C	998	2	-	0/0/11/13	0/1/1/1
2	HYP	G	998	2	-	0/0/11/13	0/1/1/1
2	HYP	F	965	2	-	0/0/11/13	0/1/1/1
2	HYP	H	995	2	-	0/0/11/13	0/1/1/1
2	HYP	C	986	2	-	0/0/11/13	0/1/1/1
2	HYP	D	971	2	-	0/0/11/13	0/1/1/1
2	HYP	D	965	2	-	0/0/11/13	0/1/1/1
2	HYP	G	986	2	-	0/0/11/13	0/1/1/1
2	HYP	C	995	2	-	0/0/11/13	0/1/1/1
2	HYP	E	971	2	-	0/0/11/13	0/1/1/1
2	HYP	F	986	2	-	0/0/11/13	0/1/1/1
2	HYP	C	1001	2	-	0/0/11/13	0/1/1/1
2	HYP	D	998	2	-	0/0/11/13	0/1/1/1
2	HYP	G	968	2	-	0/0/11/13	0/1/1/1
2	HYP	G	995	2	-	0/0/11/13	0/1/1/1
2	HYP	F	968	2	-	0/0/11/13	0/1/1/1
2	HYP	E	965	2	-	0/0/11/13	0/1/1/1
2	HYP	D	986	2	-	0/0/11/13	0/1/1/1
2	HYP	D	968	2	-	0/0/11/13	0/1/1/1
2	HYP	G	965	2	-	0/0/11/13	0/1/1/1
2	HYP	F	995	2	-	0/0/11/13	0/1/1/1
2	HYP	D	995	2	-	0/0/11/13	0/1/1/1
2	HYP	H	986	2	-	0/0/11/13	0/1/1/1
2	HYP	F	998	2	-	0/0/11/13	0/1/1/1
2	HYP	C	971	2	-	0/0/11/13	0/1/1/1
2	HYP	H	971	2	-	0/0/11/13	0/1/1/1
2	HYP	E	995	2	-	0/0/11/13	0/1/1/1
2	HYP	E	986	2	-	0/0/11/13	0/1/1/1
2	HYP	H	965	2	-	0/0/11/13	0/1/1/1
2	HYP	H	968	2	-	0/0/11/13	0/1/1/1
2	HYP	C	968	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	986	HYP	CB-CG-CD	-3.01	99.80	103.16
2	H	986	HYP	CB-CG-CD	-2.92	99.91	103.16
2	E	986	HYP	CB-CG-CD	-2.69	100.16	103.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	968	HYP	CB-CG-CD	-2.57	100.29	103.16
2	D	995	HYP	CB-CG-CD	-2.38	100.50	103.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	965	HYP	1	0
2	E	968	HYP	2	0
2	F	971	HYP	1	0
2	C	998	HYP	1	0
2	H	995	HYP	1	0
2	D	965	HYP	5	0
2	E	971	HYP	2	0
2	F	986	HYP	1	0
2	C	1001	HYP	1	0
2	D	998	HYP	1	0
2	G	968	HYP	1	0
2	G	995	HYP	1	0
2	E	965	HYP	4	0
2	F	998	HYP	2	0
2	C	971	HYP	2	0
2	H	971	HYP	4	0
2	E	986	HYP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	965:HYP	C	966:GLY	N	3.62

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	367/367 (100%)	-0.16	2 (0%) 87 72	11, 33, 54, 69	0
1	B	367/367 (100%)	-0.27	1 (0%) 90 79	9, 28, 51, 61	0
2	C	32/40 (80%)	0.52	2 (6%) 26 13	21, 51, 92, 95	0
2	D	30/40 (75%)	0.12	0 100 100	25, 38, 77, 81	0
2	E	28/40 (70%)	0.06	0 100 100	24, 44, 68, 69	0
2	F	30/40 (75%)	-0.07	0 100 100	22, 42, 81, 87	0
2	G	30/40 (75%)	-0.04	0 100 100	21, 36, 65, 77	0
2	H	28/40 (70%)	-0.21	0 100 100	13, 38, 60, 62	0
All	All	912/974 (93%)	-0.16	5 (0%) 87 72	9, 32, 60, 95	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1000	PRO	3.3
1	B	447	CYS	2.8
2	C	964	PRO	2.5
1	A	391	GLY	2.3
1	A	317	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	HYP	D	965	8/9	0.45	0.22	75,77,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HYP	C	1001	8/9	0.55	0.20	94,95,95,96	0
2	HYP	C	965	8/9	0.68	0.15	87,89,90,90	0
2	HYP	F	998	8/9	0.70	0.19	72,74,75,75	0
2	HYP	D	998	8/9	0.71	0.16	84,84,85,86	0
2	HYP	C	968	8/9	0.75	0.14	69,71,71,72	0
2	HYP	G	998	8/9	0.76	0.17	78,80,80,80	0
2	HYP	E	995	8/9	0.80	0.14	70,72,73,74	0
2	HYP	C	995	8/9	0.81	0.14	73,74,78,79	0
2	HYP	E	965	8/9	0.82	0.16	61,64,65,65	0
2	HYP	F	968	8/9	0.83	0.16	69,72,73,74	0
2	HYP	H	965	8/9	0.83	0.11	60,62,63,63	0
2	HYP	H	995	8/9	0.84	0.14	62,62,63,64	0
2	HYP	C	998	8/9	0.85	0.13	88,89,90,90	0
2	HYP	F	986	8/9	0.85	0.14	31,32,34,34	0
2	HYP	C	986	8/9	0.85	0.11	34,35,36,37	0
2	HYP	D	968	8/9	0.86	0.13	57,61,62,62	0
2	HYP	F	995	8/9	0.86	0.14	65,67,68,69	0
2	HYP	F	965	8/9	0.87	0.11	83,85,85,85	0
2	HYP	D	995	8/9	0.87	0.11	68,69,70,71	0
2	HYP	E	986	8/9	0.88	0.11	44,44,45,47	0
2	HYP	H	968	8/9	0.88	0.11	50,51,52,53	0
2	HYP	E	968	8/9	0.88	0.13	60,61,62,63	0
2	HYP	C	971	8/9	0.89	0.10	44,47,48,49	0
2	HYP	G	965	8/9	0.89	0.09	58,61,61,62	0
2	HYP	D	971	8/9	0.89	0.09	41,43,43,43	0
2	HYP	G	968	8/9	0.91	0.12	51,52,53,53	0
2	HYP	G	995	8/9	0.91	0.08	62,63,66,66	0
2	HYP	D	986	8/9	0.91	0.13	30,31,31,34	0
2	HYP	H	986	8/9	0.93	0.08	32,34,36,36	0
2	HYP	G	971	8/9	0.93	0.10	40,43,44,44	0
2	HYP	E	971	8/9	0.94	0.11	43,45,47,47	0
2	HYP	G	986	8/9	0.94	0.10	33,33,34,36	0
2	HYP	F	971	8/9	0.95	0.08	51,54,55,56	0
2	HYP	H	971	8/9	0.96	0.10	34,35,35,36	0

6.3 Carbohydrates ⓘ

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
3	CA	B	1103	1/1	0.78	0.12	95,95,95,95	0
3	CA	A	1101	1/1	0.86	0.07	68,68,68,68	0
3	CA	B	1101	1/1	0.90	0.11	70,70,70,70	0
3	CA	A	1103	1/1	0.96	0.08	63,63,63,63	0
3	CA	B	1102	1/1	0.98	0.04	31,31,31,31	0
4	ZN	A	1202	1/1	0.98	0.07	23,23,23,23	0
3	CA	A	1102	1/1	0.99	0.04	40,40,40,40	0
3	CA	B	1104	1/1	0.99	0.04	16,16,16,16	0
4	ZN	A	1201	1/1	0.99	0.02	35,35,35,35	0
3	CA	A	1104	1/1	0.99	0.02	25,25,25,25	0
4	ZN	B	1201	1/1	0.99	0.02	25,25,25,25	0
4	ZN	B	1202	1/1	0.99	0.07	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.