



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4AUO  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

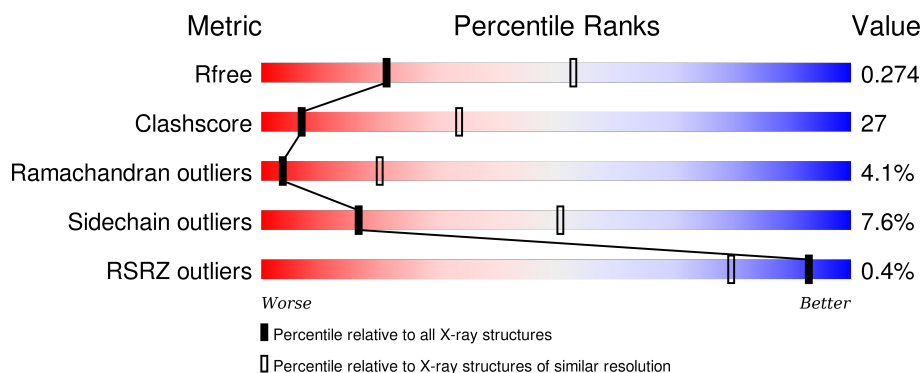
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>58%</div> <div>36%</div> <div>6%</div> </div>
1	B	367	<div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
2	C	40	<div> <div>5%</div> <div>45%</div> <div>50%</div> <div>• •</div> </div>
2	D	40	<div> <div>3%</div> <div>55%</div> <div>30%</div> <div>5%</div> <div>10%</div> </div>
2	E	40	<div> <div>38%</div> <div>38%</div> <div>8%</div> <div>18%</div> </div>

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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 (three-letter code: CA) (formula: Ca).

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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

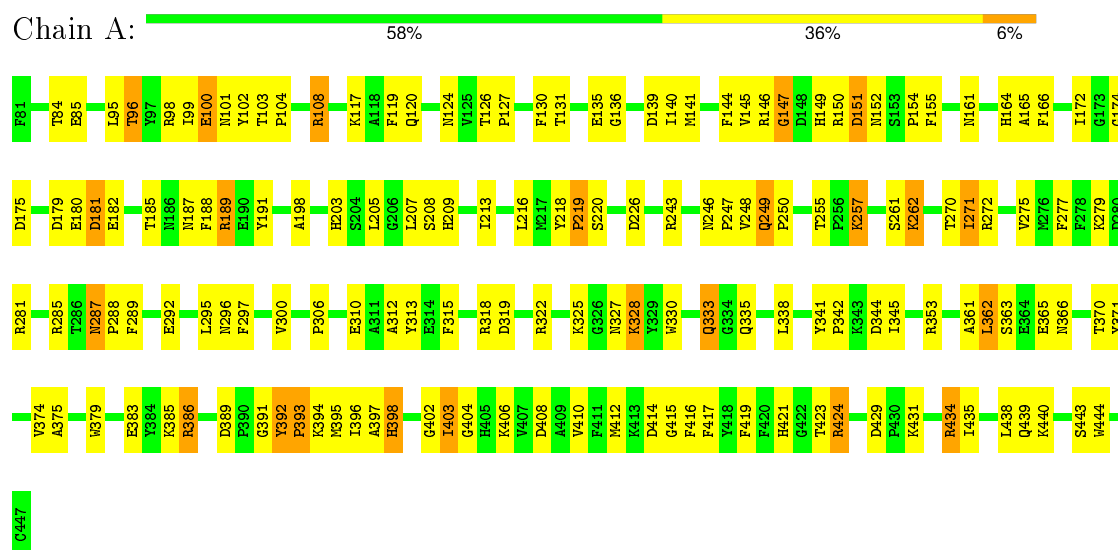
- Molecule 5 is water.

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

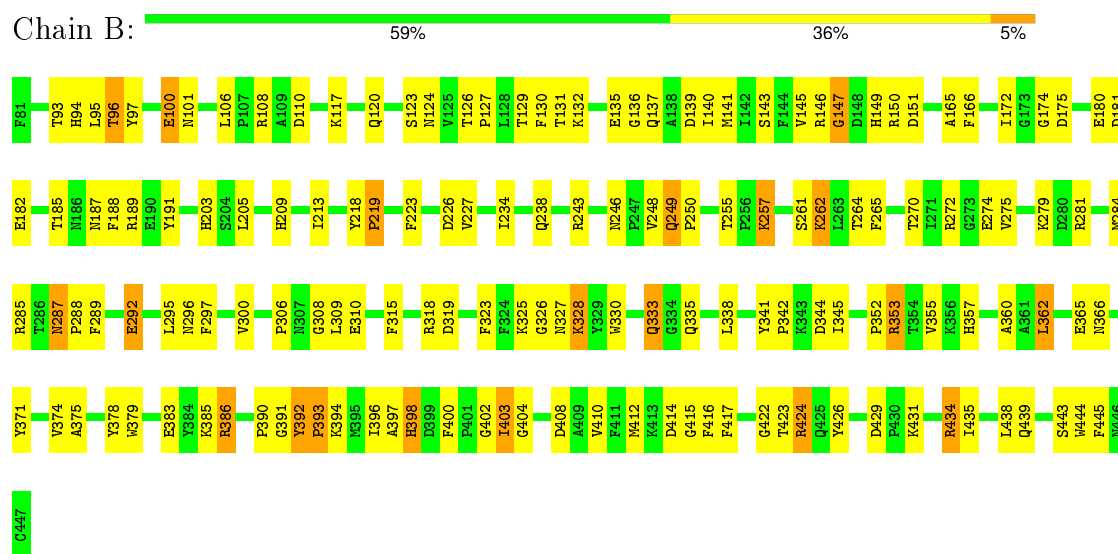
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

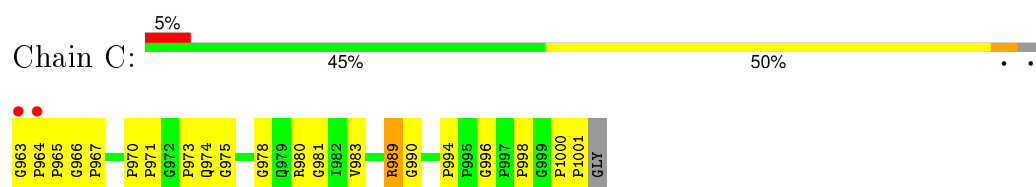
#### • Molecule 1: INTERSTITIAL COLLAGENASE



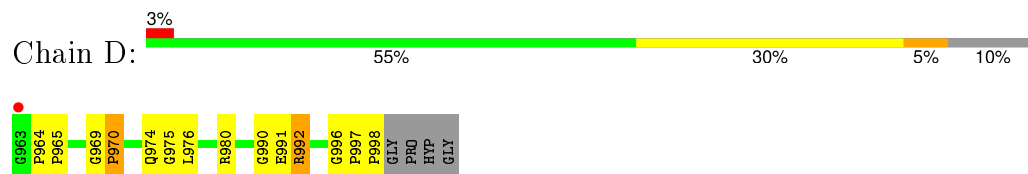
#### • Molecule 1: INTERSTITIAL COLLAGENASE



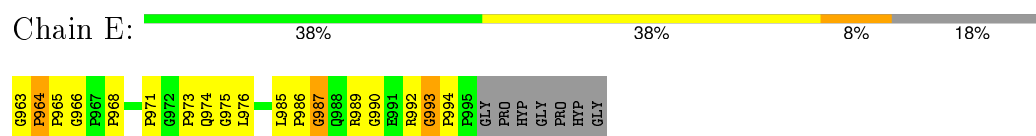
#### • Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



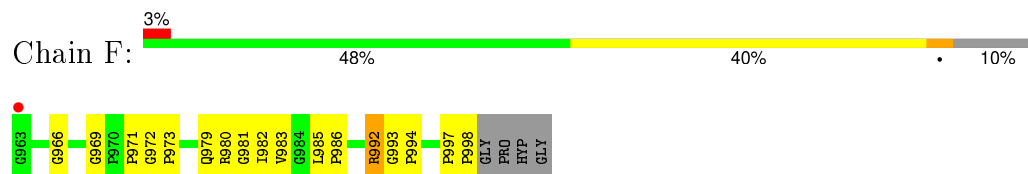
- Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



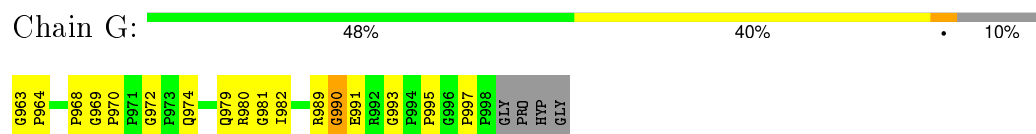
- Molecule 2: TRIPLE-HELICAL COLLAGEN PEPTIDE



- 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, $\alpha$ , $\beta$ , $\gamma$	76.67Å 102.24Å 80.73Å 90.00° 103.75° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.00-3.00) 86.5 (19.90-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 20982 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HYP, ZN, CA

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	0.45	0/3086	0.65	0/4188
1	B	0.45	0/3085	0.66	0/4187
2	C	0.41	0/202	0.75	0/263
2	D	0.39	0/195	0.68	0/254
2	E	0.36	0/170	0.66	0/223
2	F	0.37	0/191	0.76	0/249
2	G	0.40	0/189	0.72	0/247
2	H	0.36	0/170	0.61	0/223
All	All	0.44	0/7288	0.66	0/9834

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 [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	160	0
1	B	2985	0	2799	144	0
2	C	258	0	248	26	0
2	D	243	0	235	18	0
2	E	210	0	196	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	239	0	231	22	0
2	G	237	0	224	20	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	383	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 27.

All (383) 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:HH11	1:B:386:ARG:HB3	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
2:D:965:HYP:HA	2:E:964:PRO:HD2	1.53	0.91
2:C:967:PRO:HG2	2:E:965:HYP:HA	1.52	0.89
1:A:403:ILE:HD12	1:A:404:GLY:N	1.85	0.89
1:B:287:ASN:HD22	1:B:288:PRO:HD2	1.38	0.88
1:A:287:ASN:HD22	1:A:288:PRO:CD	1.87	0.88
1:A:246:ASN:HD21	1:A:248:VAL:HG23	1.38	0.87
1:A:386:ARG:HH11	1:A:386:ARG:HB3	1.39	0.87
1:B:287:ASN:HD22	1:B:288:PRO:CD	1.89	0.86
1:A:145:VAL:HG21	1:A:149:HIS:CD2	2.13	0.83
1:A:246:ASN:HD21	1:A:248:VAL:CG2	1.91	0.83
2:F:973:PRO:HG2	2:H:971:HYP:OD1	1.79	0.83
1:A:333:GLN:HB2	1:A:338:LEU:HD21	1.61	0.82
1:B:246:ASN:HD21	1:B:248:VAL:HG23	1.43	0.81
1:A:287:ASN:HD22	1:A:288:PRO:HD2	1.43	0.81
1:A:243:ARG:HG2	1:A:243:ARG:HH11	1.46	0.80
1:B:261:SER:O	1:B:262:LYS:HB2	1.82	0.80
1:B:145:VAL:HG21	1:B:149:HIS:CD2	2.16	0.79
2:C:971:HYP:HA	2:D:970:PRO:HD2	1.64	0.79
1:A:209:HIS:CG	1:A:219:PRO:HG3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:PHE:CD1	2:E:971:HYP:HG	2.19	0.77
2:F:992:ARG:HG3	2:G:991:GLU:HB2	1.64	0.77
1:A:392:TYR:O	1:A:394:LYS:N	2.17	0.76
1:B:246:ASN:ND2	1:B:249:GLN:H	1.84	0.76
1:B:392:TYR:O	1:B:394:LYS:N	2.19	0.76
1:B:130:PHE:HZ	1:B:205:LEU:HD21	1.52	0.75
1:A:379:TRP:CZ3	1:A:393:PRO:HG3	2.22	0.74
2:C:989:ARG:HD2	2:D:990:GLY:HA2	1.67	0.74
2:C:989:ARG:HG3	2:C:990:GLY:N	2.02	0.73
1:A:287:ASN:HD22	1:A:288:PRO:N	1.87	0.73
1:A:213:ILE:HD12	1:A:296:ASN:HA	1.70	0.73
1:B:310:GLU:HG3	1:B:325:LYS:HA	1.71	0.73
1:B:246:ASN:HD21	1:B:248:VAL:CG2	2.03	0.72
1:B:362:LEU:HD13	1:B:362:LEU:O	1.90	0.72
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.56	0.71
1:B:100:GLU:OE2	1:B:141:MET:HB3	1.91	0.70
1:B:243:ARG:HH11	1:B:243:ARG:HG2	1.56	0.70
1:B:379:TRP:CZ3	1:B:393:PRO:HG3	2.27	0.70
1:B:187:ASN:HD21	1:B:189:ARG:CG	2.05	0.70
2:C:980:ARG:HG2	2:C:981:GLY:N	2.06	0.70
1:A:102:TYR:CD2	1:A:108:ARG:HG2	2.27	0.69
2:F:994:PRO:HG3	2:H:989:ARG:CZ	2.23	0.69
1:B:287:ASN:ND2	1:B:288:PRO:HD2	2.08	0.69
2:F:998:HYP:HA	2:G:997:PRO:O	1.91	0.68
2:G:963:GLY:N	2:G:964:PRO:HD3	2.08	0.68
1:B:97:TYR:CZ	1:B:132:LYS:HB2	2.29	0.68
1:A:261:SER:O	1:A:262:LYS:HB2	1.93	0.68
1:A:270:THR:HG22	1:A:275:VAL:HG22	1.76	0.67
1:A:246:ASN:ND2	1:A:249:GLN:H	1.93	0.67
1:B:126:THR:HB	1:B:127:PRO:HD2	1.77	0.67
2:D:974:GLN:OE1	2:E:973:PRO:HG2	1.94	0.67
1:B:165:ALA:HA	1:B:175:ASP:O	1.95	0.67
1:B:365:GLU:HG3	1:B:366:ASN:OD1	1.96	0.66
1:A:315:PHE:CZ	1:A:383:GLU:HB3	2.31	0.66
2:G:963:GLY:HA2	2:H:963:GLY:HA2	1.76	0.66
1:A:96:THR:HG23	1:A:139:ASP:OD2	1.96	0.66
1:A:161:ASN:ND2	2:E:974:GLN:HG2	2.11	0.66
1:A:403:ILE:N	1:A:435:ILE:HD11	2.12	0.65
1:A:287:ASN:ND2	1:A:288:PRO:HD2	2.11	0.65
1:A:310:GLU:HG3	1:A:325:LYS:HA	1.79	0.64
1:B:246:ASN:OD1	1:B:248:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASN:HD21	1:B:189:ARG:HG3	1.63	0.64
1:B:130:PHE:CZ	1:B:205:LEU:HD21	2.33	0.63
1:B:328:LYS:HG3	1:B:342:PRO:HB2	1.79	0.63
1:A:379:TRP:CH2	1:A:393:PRO:HG3	2.33	0.63
2:F:972:GLY:HA3	2:H:969:GLY:O	1.98	0.63
1:B:187:ASN:ND2	1:B:189:ARG:HG3	2.14	0.63
1:A:246:ASN:OD1	1:A:248:VAL:HG22	1.98	0.63
1:A:365:GLU:HG3	1:A:366:ASN:OD1	1.98	0.63
2:G:980:ARG:HG3	2:G:981:GLY:H	1.64	0.63
1:A:438:LEU:HD13	1:A:439:GLN:N	2.13	0.63
2:F:980:ARG:CG	2:F:981:GLY:H	2.13	0.62
2:D:965:HYP:OD1	2:E:964:PRO:HG2	2.00	0.62
1:B:209:HIS:CG	1:B:219:PRO:HG3	2.35	0.62
1:A:135:GLU:HG2	1:A:136:GLY:N	2.14	0.62
1:A:255:THR:O	1:A:257:LYS:HE2	1.99	0.62
1:B:255:THR:O	1:B:257:LYS:HE2	2.00	0.61
1:B:315:PHE:HE2	1:B:318:ARG:HD3	1.65	0.61
1:A:126:THR:HB	1:A:127:PRO:HD2	1.82	0.61
2:G:995:HYP:OD1	2:H:994:PRO:HD2	2.01	0.60
2:D:965:HYP:CA	2:E:964:PRO:HD2	2.29	0.60
2:F:980:ARG:HG2	2:F:981:GLY:N	2.17	0.60
1:B:270:THR:HG22	1:B:275:VAL:HG22	1.83	0.60
1:B:96:THR:HA	1:B:131:THR:O	2.02	0.59
1:A:386:ARG:HH11	1:A:386:ARG:CB	2.14	0.59
1:B:429:ASP:OD1	1:B:431:LYS:HD2	2.02	0.59
1:B:287:ASN:HD22	1:B:288:PRO:N	2.00	0.59
1:A:429:ASP:OD1	1:A:431:LYS:HD2	2.01	0.59
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.68	0.59
1:B:434:ARG:HG2	1:B:434:ARG:HH11	1.68	0.59
1:B:315:PHE:CE2	1:B:318:ARG:HD3	2.38	0.58
2:C:994:PRO:HG3	2:E:989:ARG:CZ	2.32	0.58
2:F:980:ARG:CG	2:F:981:GLY:N	2.66	0.58
1:A:257:LYS:N	1:A:257:LYS:HE3	2.18	0.58
1:A:262:LYS:NZ	1:A:423:THR:HG21	2.17	0.58
2:F:971:HYP:HA	2:G:970:PRO:HD2	1.85	0.58
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.68	0.58
1:B:362:LEU:CD1	1:B:371:TYR:HB2	2.34	0.58
1:A:140:ILE:HG23	1:A:174:GLY:O	2.02	0.58
1:A:213:ILE:HD11	1:A:295:LEU:HG	1.85	0.58
1:B:327:ASN:O	1:B:345:ILE:HG12	2.03	0.58
1:B:300:VAL:HG11	2:G:982:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:H	1:B:257:LYS:HE3	1.69	0.57
1:A:362:LEU:O	1:A:362:LEU:HD13	2.03	0.57
1:A:257:LYS:H	1:A:257:LYS:HE3	1.70	0.57
1:B:403:ILE:CD1	1:B:404:GLY:N	2.63	0.57
1:B:185:THR:HB	1:B:187:ASN:OD1	2.05	0.56
1:A:166:PHE:CE2	1:A:172:ILE:HD11	2.41	0.56
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.19	0.56
1:A:180:GLU:C	1:A:182:GLU:H	2.07	0.56
2:D:996:GLY:O	2:D:998:HYP:HD23	2.06	0.56
1:A:130:PHE:CZ	1:A:205:LEU:HD21	2.40	0.56
1:B:365:GLU:HG3	1:B:366:ASN:H	1.70	0.56
1:B:257:LYS:HE3	1:B:257:LYS:N	2.19	0.56
1:A:100:GLU:OE2	1:A:141:MET:HB3	2.06	0.56
2:C:980:ARG:CG	2:C:981:GLY:N	2.69	0.56
2:C:980:ARG:HG2	2:C:981:GLY:H	1.68	0.56
1:A:96:THR:HA	1:A:131:THR:O	2.06	0.56
1:A:330:TRP:CE2	1:A:342:PRO:HB3	2.41	0.56
1:A:403:ILE:H	1:A:435:ILE:HD11	1.71	0.56
1:A:306:PRO:HG3	1:A:330:TRP:CH2	2.40	0.56
1:A:353:ARG:HH11	1:A:353:ARG:HB3	1.71	0.56
1:B:438:LEU:HD13	1:B:439:GLN:N	2.21	0.56
1:A:327:ASN:O	1:A:345:ILE:HG12	2.05	0.55
1:B:140:ILE:HG23	1:B:174:GLY:O	2.06	0.55
1:B:379:TRP:N	1:B:379:TRP:CD1	2.73	0.55
1:A:130:PHE:HZ	1:A:205:LEU:HD21	1.71	0.55
1:A:289:PHE:CD2	2:E:985:LEU:HD22	2.42	0.55
1:B:262:LYS:NZ	1:B:423:THR:HG21	2.22	0.55
2:F:980:ARG:HG2	2:F:981:GLY:H	1.71	0.55
2:C:964:PRO:C	2:D:964:PRO:HD2	2.26	0.55
2:F:973:PRO:O	2:H:971:HYP:HA	2.07	0.55
1:B:213:ILE:HD12	1:B:296:ASN:HA	1.89	0.55
1:A:341:TYR:HB3	1:A:342:PRO:HA	1.89	0.55
1:B:146:ARG:HG2	1:B:146:ARG:NH1	2.22	0.54
1:B:172:ILE:HG12	1:B:172:ILE:O	2.07	0.54
1:B:360:ALA:HB1	1:B:410:VAL:HG12	1.89	0.54
1:A:365:GLU:HG3	1:A:366:ASN:H	1.71	0.54
1:B:386:ARG:HH11	1:B:386:ARG:CB	2.10	0.54
1:B:352:PRO:CD	1:B:379:TRP:CH2	2.91	0.54
1:B:213:ILE:HD11	1:B:295:LEU:HG	1.89	0.54
2:D:965:HYP:HA	2:E:964:PRO:CD	2.32	0.54
2:C:994:PRO:HG3	2:E:989:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:PHE:CE2	1:A:318:ARG:HD3	2.42	0.54
1:A:152:ASN:O	2:E:973:PRO:HB3	2.08	0.54
1:A:325:LYS:HB3	1:A:330:TRP:HZ3	1.74	0.53
1:A:180:GLU:O	1:A:182:GLU:N	2.41	0.53
1:A:185:THR:HB	1:A:187:ASN:OD1	2.08	0.53
1:B:378:TYR:C	1:B:379:TRP:CD1	2.82	0.53
1:A:424:ARG:HB2	1:A:438:LEU:HD21	1.90	0.53
1:A:95:LEU:HD12	1:A:130:PHE:CE1	2.43	0.53
2:H:976:LEU:HD23	2:H:977:ALA:N	2.24	0.53
1:A:402:GLY:O	1:A:404:GLY:N	2.42	0.53
2:E:965:HYP:O	2:E:966:GLY:HA3	2.09	0.53
1:A:246:ASN:ND2	1:A:248:VAL:CG2	2.69	0.52
2:F:994:PRO:O	2:G:993:GLY:HA3	2.09	0.52
1:A:135:GLU:HG2	1:A:136:GLY:H	1.74	0.52
1:B:146:ARG:O	1:B:147:GLY:C	2.48	0.52
1:A:165:ALA:HA	1:A:175:ASP:O	2.09	0.52
1:B:412:MET:SD	1:B:417:PHE:HE1	2.33	0.52
1:B:315:PHE:CZ	1:B:383:GLU:HB3	2.44	0.52
2:G:974:GLN:HE21	2:H:975:GLY:HA2	1.73	0.52
2:C:998:HYP:OD1	2:D:997:PRO:HG2	2.09	0.52
1:B:330:TRP:CE2	1:B:342:PRO:HB3	2.45	0.52
2:G:989:ARG:HG3	2:G:990:GLY:N	2.25	0.52
1:A:120:GLN:HG2	1:A:124:ASN:ND2	2.25	0.52
1:A:379:TRP:N	1:A:379:TRP:CD1	2.78	0.52
1:B:328:LYS:HB3	1:B:328:LYS:NZ	2.25	0.52
1:B:297:PHE:O	1:B:300:VAL:HG23	2.09	0.52
2:C:967:PRO:CG	2:E:965:HYP:HA	2.31	0.51
1:A:243:ARG:CG	1:A:243:ARG:HH11	2.18	0.51
1:B:106:LEU:HD22	1:B:110:ASP:HB3	1.91	0.51
1:B:166:PHE:CZ	1:B:172:ILE:HD11	2.46	0.51
1:B:402:GLY:HA3	1:B:435:ILE:HD11	1.92	0.51
2:F:973:PRO:HG2	2:H:971:HYP:HD1	1.73	0.51
2:C:980:ARG:CG	2:C:981:GLY:H	2.22	0.51
2:C:978:GLY:HA3	2:E:976:LEU:O	2.11	0.51
1:A:108:ARG:NH1	1:A:108:ARG:HG3	2.25	0.51
1:A:403:ILE:HG21	1:A:419:PHE:CD2	2.46	0.51
2:C:970:PRO:O	2:D:969:GLY:HA3	2.11	0.51
2:C:964:PRO:O	2:D:964:PRO:HD2	2.10	0.50
1:B:187:ASN:HD21	1:B:189:ARG:HD2	1.76	0.50
1:A:362:LEU:HD21	1:A:417:PHE:CZ	2.45	0.50
1:A:145:VAL:HG21	1:A:149:HIS:NE2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HE2	1:A:262:LYS:CA	2.42	0.50
1:B:264:THR:HG22	1:B:422:GLY:O	2.11	0.50
1:B:187:ASN:HD21	1:B:189:ARG:CD	2.24	0.50
1:A:117:LYS:O	1:A:120:GLN:HB3	2.12	0.50
1:A:287:ASN:ND2	1:A:288:PRO:N	2.58	0.50
1:B:379:TRP:CH2	1:B:393:PRO:HG3	2.46	0.50
1:B:402:GLY:O	1:B:404:GLY:N	2.45	0.50
1:B:166:PHE:CE1	1:B:172:ILE:HD11	2.47	0.50
1:A:248:VAL:O	1:A:249:GLN:CB	2.60	0.49
1:A:325:LYS:HB3	1:A:330:TRP:CZ3	2.47	0.49
1:B:424:ARG:NH1	1:B:426:TYR:OH	2.42	0.49
2:C:996:GLY:HA3	2:E:994:PRO:O	2.12	0.49
2:G:980:ARG:CG	2:G:981:GLY:N	2.75	0.49
1:A:180:GLU:C	1:A:182:GLU:N	2.66	0.49
1:A:218:TYR:O	1:A:220:SER:N	2.41	0.49
1:A:297:PHE:O	1:A:300:VAL:HG23	2.12	0.49
1:B:309:LEU:HD13	1:B:323:PHE:CD1	2.47	0.49
1:B:443:SER:O	1:B:445:PHE:N	2.46	0.49
1:B:248:VAL:O	1:B:249:GLN:CB	2.61	0.49
1:B:264:THR:O	1:B:279:LYS:HD3	2.13	0.49
1:A:246:ASN:HD21	1:A:248:VAL:HG22	1.77	0.48
1:A:246:ASN:HD22	1:A:250:PRO:HD3	1.78	0.48
1:B:101:ASN:OD1	1:B:143:SER:HB2	2.12	0.48
1:B:234:ILE:O	1:B:238:GLN:HG3	2.13	0.48
1:B:180:GLU:C	1:B:182:GLU:H	2.16	0.48
1:B:365:GLU:HG3	1:B:366:ASN:N	2.28	0.48
1:A:353:ARG:NH1	1:A:353:ARG:HB3	2.28	0.48
1:B:243:ARG:NH1	1:B:243:ARG:HG2	2.24	0.48
1:A:151:ASP:O	1:A:152:ASN:CB	2.62	0.48
2:F:972:GLY:O	2:G:972:GLY:HA2	2.13	0.48
1:B:353:ARG:HH11	1:B:353:ARG:HB3	1.78	0.48
1:A:198:ALA:HB1	1:A:216:LEU:HD21	1.96	0.48
1:B:306:PRO:HG3	1:B:330:TRP:CH2	2.48	0.48
1:A:257:LYS:N	1:A:257:LYS:CE	2.75	0.48
1:A:386:ARG:NH1	1:A:386:ARG:HB3	2.17	0.48
1:B:434:ARG:NH1	1:B:434:ARG:HG2	2.29	0.48
1:B:96:THR:HG23	1:B:139:ASP:OD2	2.14	0.47
1:A:440:LYS:O	1:A:443:SER:HB3	2.13	0.47
2:F:992:ARG:HG2	2:F:993:GLY:N	2.29	0.47
1:A:270:THR:O	1:A:271:ILE:C	2.51	0.47
1:A:341:TYR:HA	1:A:342:PRO:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HH11	1:A:424:ARG:HG3	1.78	0.47
2:C:973:PRO:HD2	2:E:971:HYP:HA	1.95	0.47
1:A:103:THR:HB	1:A:144:PHE:CD2	2.49	0.47
1:B:135:GLU:HG2	1:B:136:GLY:N	2.29	0.47
2:C:971:HYP:O	2:E:968:HYP:O	2.33	0.47
1:B:146:ARG:HG3	1:B:180:GLU:HB3	1.97	0.47
1:A:403:ILE:CD1	1:A:404:GLY:N	2.69	0.47
2:C:963:GLY:N	2:C:964:PRO:HD2	2.29	0.47
1:A:209:HIS:ND1	1:A:219:PRO:HG3	2.29	0.47
1:A:306:PRO:HG3	1:A:330:TRP:CZ3	2.49	0.47
1:A:362:LEU:HD23	1:A:412:MET:HB2	1.97	0.47
1:B:257:LYS:CE	1:B:257:LYS:N	2.77	0.47
1:A:146:ARG:O	1:A:147:GLY:C	2.53	0.47
1:A:335:GLN:O	1:A:335:GLN:HG2	2.15	0.47
1:B:262:LYS:HA	1:B:423:THR:HG21	1.95	0.47
2:D:976:LEU:O	2:E:975:GLY:HA3	2.15	0.47
1:B:218:TYR:OH	2:G:979:GLN:NE2	2.46	0.47
1:A:365:GLU:HG3	1:A:366:ASN:N	2.29	0.47
1:A:243:ARG:NH1	1:A:243:ARG:HG2	2.22	0.46
2:D:974:GLN:HG3	2:D:975:GLY:N	2.30	0.46
1:A:146:ARG:NH1	1:A:181:ASP:OD1	2.48	0.46
1:A:99:ILE:O	1:A:100:GLU:C	2.54	0.46
1:B:318:ARG:O	1:B:319:ASP:C	2.52	0.46
1:B:403:ILE:N	1:B:435:ILE:HD11	2.31	0.46
1:A:145:VAL:HG21	1:A:149:HIS:CG	2.49	0.46
1:B:262:LYS:CA	1:B:262:LYS:HE2	2.46	0.46
2:G:970:PRO:O	2:H:969:GLY:HA3	2.15	0.46
1:B:327:ASN:O	1:B:345:ILE:HG23	2.15	0.46
1:A:315:PHE:HE2	1:A:318:ARG:HD3	1.79	0.46
1:A:328:LYS:HG3	1:A:342:PRO:HB2	1.97	0.46
1:A:146:ARG:HG3	1:A:180:GLU:HB3	1.97	0.46
1:B:438:LEU:HD13	1:B:438:LEU:C	2.36	0.46
1:B:352:PRO:HG2	1:B:379:TRP:HH2	1.80	0.46
1:B:262:LYS:HA	1:B:423:THR:CG2	2.47	0.45
1:B:135:GLU:HG2	1:B:136:GLY:H	1.81	0.45
1:B:426:TYR:CE1	1:B:438:LEU:HD23	2.51	0.45
1:B:120:GLN:HG2	1:B:124:ASN:ND2	2.31	0.45
2:G:968:HYP:HA	2:H:967:PRO:HD2	1.97	0.45
1:B:386:ARG:NH1	1:B:386:ARG:HB3	2.15	0.45
1:B:365:GLU:CA	1:B:412:MET:HE3	2.46	0.45
1:B:335:GLN:O	1:B:335:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:964:PRO:HA	2:C:965:HYP:HD23	1.81	0.45
1:A:187:ASN:HD21	1:A:189:ARG:CG	2.30	0.45
2:F:997:PRO:CG	2:H:995:HYP:OD1	2.64	0.45
1:B:145:VAL:HG21	1:B:149:HIS:CG	2.51	0.45
1:B:306:PRO:HG3	1:B:330:TRP:CZ3	2.52	0.45
1:B:326:GLY:O	1:B:357:HIS:HA	2.16	0.45
1:B:146:ARG:NH1	1:B:181:ASP:OD1	2.50	0.45
1:B:117:LYS:O	1:B:120:GLN:HB3	2.16	0.45
2:H:970:PRO:HA	2:H:971:HYP:HD23	1.84	0.45
2:G:990:GLY:C	2:G:991:GLU:HG3	2.37	0.45
1:B:95:LEU:HD12	1:B:130:PHE:CE1	2.51	0.45
1:B:341:TYR:HA	1:B:342:PRO:C	2.37	0.45
1:A:84:THR:HA	1:A:208:SER:OG	2.17	0.45
1:A:306:PRO:HD3	1:A:330:TRP:CE2	2.52	0.45
1:A:406:LYS:O	1:A:421:HIS:CD2	2.70	0.45
1:A:262:LYS:HA	1:A:262:LYS:HE2	1.99	0.44
1:A:246:ASN:ND2	1:A:248:VAL:HG22	2.32	0.44
1:A:164:HIS:HB3	2:E:974:GLN:OE1	2.17	0.44
2:G:980:ARG:HG3	2:G:981:GLY:N	2.30	0.44
1:B:402:GLY:HA3	1:B:435:ILE:CD1	2.48	0.44
1:A:262:LYS:N	1:A:262:LYS:HE2	2.33	0.44
1:A:277:PHE:N	1:A:277:PHE:CD1	2.86	0.44
1:B:330:TRP:CZ2	1:B:342:PRO:HB3	2.52	0.44
1:A:119:PHE:CD1	1:A:130:PHE:CG	3.06	0.44
1:A:248:VAL:O	1:A:249:GLN:HB3	2.18	0.44
1:B:180:GLU:C	1:B:182:GLU:N	2.71	0.44
1:A:126:THR:HB	1:A:127:PRO:CD	2.44	0.44
1:B:414:ASP:C	1:B:416:PHE:H	2.21	0.44
1:A:412:MET:HE2	1:A:412:MET:HB3	1.75	0.43
1:A:261:SER:O	1:A:262:LYS:CB	2.65	0.43
2:C:975:GLY:HA3	2:E:973:PRO:O	2.17	0.43
1:A:287:ASN:ND2	1:A:287:ASN:C	2.72	0.43
1:B:132:LYS:HG2	1:B:132:LYS:O	2.18	0.43
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.83	0.43
1:A:289:PHE:HD2	2:E:985:LEU:CD2	2.32	0.43
2:D:964:PRO:HA	2:D:965:HYP:HD23	1.87	0.43
1:A:246:ASN:OD1	1:A:247:PRO:HD2	2.18	0.43
1:A:318:ARG:O	1:A:319:ASP:C	2.56	0.43
1:B:218:TYR:HA	1:B:219:PRO:HD3	1.82	0.43
1:B:355:VAL:HG13	1:B:374:VAL:HG11	2.01	0.43
1:B:94:HIS:CE1	1:B:129:THR:HG21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:PHE:O	1:B:403:ILE:HG13	2.18	0.43
1:A:328:LYS:NZ	1:A:328:LYS:HB3	2.33	0.43
2:E:986:HYP:O	2:E:987:GLY:O	2.36	0.43
1:B:352:PRO:HD3	1:B:379:TRP:CZ3	2.53	0.43
1:B:223:PHE:HE1	1:B:227:VAL:HG23	1.83	0.43
1:B:265:PHE:HE1	1:B:284:MET:CE	2.30	0.43
2:F:994:PRO:HG3	2:H:989:ARG:NH2	2.33	0.43
2:C:974:GLN:O	2:C:975:GLY:C	2.56	0.43
1:A:313:TYR:CZ	1:A:370:THR:HG21	2.54	0.43
1:B:279:LYS:HD2	1:B:279:LYS:HA	1.71	0.42
1:A:84:THR:HG22	1:A:85:GLU:N	2.34	0.42
1:A:374:VAL:O	1:A:375:ALA:HB3	2.19	0.42
1:A:438:LEU:HD13	1:A:438:LEU:C	2.39	0.42
1:A:287:ASN:C	1:A:287:ASN:HD22	2.19	0.42
1:B:246:ASN:HD22	1:B:250:PRO:HD3	1.84	0.42
1:A:98:ARG:NH1	1:A:136:GLY:O	2.50	0.42
2:D:964:PRO:O	2:E:963:GLY:HA3	2.18	0.42
1:B:365:GLU:N	1:B:412:MET:CE	2.83	0.42
1:A:365:GLU:HA	1:A:412:MET:HE3	2.01	0.42
1:A:95:LEU:HD12	1:A:130:PHE:HE1	1.84	0.42
1:A:363:SER:HA	1:A:370:THR:HA	2.01	0.42
2:E:964:PRO:O	2:E:965:HYP:O	2.38	0.42
1:B:412:MET:HB3	1:B:412:MET:HE2	1.76	0.42
2:G:989:ARG:O	2:G:990:GLY:O	2.38	0.42
1:B:308:GLY:O	1:B:325:LYS:HE3	2.18	0.42
1:A:414:ASP:C	1:A:416:PHE:H	2.23	0.42
1:B:402:GLY:O	1:B:403:ILE:C	2.57	0.42
1:A:362:LEU:HB3	1:A:410:VAL:HG13	2.00	0.42
1:A:402:GLY:O	1:A:403:ILE:C	2.58	0.42
1:A:101:ASN:HD21	1:A:144:PHE:HB2	1.85	0.42
1:A:103:THR:HA	1:A:104:PRO:HD3	1.85	0.42
1:A:279:LYS:HA	1:A:279:LYS:HD2	1.65	0.42
1:A:330:TRP:CZ2	1:A:342:PRO:HB3	2.55	0.42
1:A:289:PHE:CD2	2:E:985:LEU:CD2	3.03	0.42
1:B:209:HIS:ND1	1:B:219:PRO:HG3	2.35	0.41
2:D:992:ARG:HH11	2:D:992:ARG:HG3	1.85	0.41
2:D:974:GLN:HG3	2:D:975:GLY:O	2.20	0.41
2:H:976:LEU:HD23	2:H:977:ALA:H	1.83	0.41
1:B:120:GLN:HA	1:B:123:SER:OG	2.20	0.41
2:C:966:GLY:HA3	2:E:963:GLY:C	2.41	0.41
2:C:970:PRO:HG2	2:E:968:HYP:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:SER:C	1:B:445:PHE:H	2.23	0.41
2:F:969:GLY:HA3	2:H:966:GLY:O	2.20	0.41
1:A:172:ILE:HG12	1:A:172:ILE:O	2.19	0.41
1:B:165:ALA:HB3	1:B:203:HIS:HB2	2.03	0.41
1:A:203:HIS:HA	1:A:207:LEU:O	2.20	0.41
1:A:312:ALA:HA	1:A:322:ARG:O	2.20	0.41
1:B:396:ILE:C	1:B:398:HIS:H	2.24	0.41
1:B:292:GLU:O	1:B:292:GLU:OE2	2.38	0.41
1:B:219:PRO:O	2:F:980:ARG:HB2	2.20	0.41
1:A:155:PHE:CD1	1:A:179:ASP:HB2	2.56	0.41
1:A:402:GLY:HA3	1:A:435:ILE:CD1	2.50	0.41
1:A:396:ILE:C	1:A:398:HIS:H	2.24	0.41
1:B:137:GLN:HA	1:B:137:GLN:OE1	2.21	0.41
1:A:361:ALA:HA	1:A:371:TYR:O	2.21	0.41
1:A:289:PHE:CE2	2:E:985:LEU:HD22	2.55	0.41
1:A:84:THR:HG22	1:A:85:GLU:O	2.21	0.41
2:E:992:ARG:O	2:E:993:GLY:O	2.39	0.41
2:F:985:LEU:HA	2:F:986:HYP:HD23	1.83	0.41
1:A:152:ASN:C	1:A:154:PRO:HD3	2.42	0.41
1:A:99:ILE:O	1:A:99:ILE:HG22	2.21	0.41
1:A:385:LYS:HB3	1:A:385:LYS:HE2	1.92	0.40
1:B:385:LYS:HE2	1:B:385:LYS:HB3	1.92	0.40
2:C:1000:PRO:HA	2:C:1001:HYP:HD23	1.90	0.40
1:B:374:VAL:O	1:B:375:ALA:HB3	2.21	0.40
2:F:966:GLY:HA3	2:H:964:PRO:O	2.21	0.40
1:A:218:TYR:HA	1:A:219:PRO:HD3	1.79	0.40
2:F:998:HYP:OD1	2:G:997:PRO:HG2	2.22	0.40
1:A:362:LEU:CD1	1:A:371:TYR:HB2	2.52	0.40
2:E:989:ARG:HG2	2:E:990:GLY:N	2.36	0.40
1:B:108:ARG:HB3	1:B:108:ARG:HE	1.62	0.40
1:B:289:PHE:CD1	1:B:289:PHE:N	2.88	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	365/367 (100%)	318 (87%)	31 (8%)	16 (4%)	3	18
1	B	365/367 (100%)	316 (87%)	37 (10%)	12 (3%)	5	26
2	C	31/40 (78%)	28 (90%)	2 (6%)	1 (3%)	5	27
2	D	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	7
2	E	26/40 (65%)	20 (77%)	3 (12%)	3 (12%)	0	2
2	F	29/40 (72%)	25 (86%)	3 (10%)	1 (3%)	5	25
2	G	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	7
2	H	27/40 (68%)	22 (82%)	5 (18%)	0	100	100
All	All	901/974 (92%)	775 (86%)	89 (10%)	37 (4%)	3	20

All (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
1	A	391	GLY
1	A	397	ALA
1	B	147	GLY
1	B	272	ARG
1	B	397	ALA
1	B	444	TRP
2	E	987	GLY
2	E	993	GLY
2	F	992	ARG
2	G	990	GLY
1	A	100	GLU
1	A	108	ARG
1	A	181	ASP
1	B	100	GLU
1	A	191	TYR
1	A	219	PRO
1	A	249	GLN
1	A	272	ARG
1	B	191	TYR

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Mol	Chain	Res	Type
1	B	249	GLN
1	B	391	GLY
1	A	444	TRP
2	C	983	VAL
2	D	970	PRO
2	D	980	ARG
1	B	393	PRO
1	A	415	GLY
1	A	393	PRO
1	B	415	GLY
2	E	964	PRO
1	A	271	ILE
1	B	219	PRO

### 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%)	288 (93%)	23 (7%)	17	52
1	B	311/313 (99%)	286 (92%)	25 (8%)	15	47
2	C	17/18 (94%)	16 (94%)	1 (6%)	24	63
2	D	17/18 (94%)	15 (88%)	2 (12%)	6	26
2	E	13/18 (72%)	13 (100%)	0	100	100
2	F	16/18 (89%)	13 (81%)	3 (19%)	2	10
2	G	16/18 (89%)	16 (100%)	0	100	100
2	H	13/18 (72%)	13 (100%)	0	100	100
All	All	714/734 (97%)	660 (92%)	54 (8%)	16	51

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	THR
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	151	ASP
1	A	188	PHE
1	A	226	ASP
1	A	257	LYS
1	A	262	LYS
1	A	281	ARG
1	A	285	ARG
1	A	287	ASN
1	A	292	GLU
1	A	328	LYS
1	A	333	GLN
1	A	344	ASP
1	A	362	LEU
1	A	386	ARG
1	A	389	ASP
1	A	392	TYR
1	A	395	MET
1	A	398	HIS
1	A	408	ASP
1	A	424	ARG
1	A	434	ARG
1	B	93	THR
1	B	96	THR
1	B	150	ARG
1	B	151	ASP
1	B	188	PHE
1	B	226	ASP
1	B	257	LYS
1	B	262	LYS
1	B	274	GLU
1	B	281	ARG
1	B	285	ARG
1	B	287	ASN
1	B	292	GLU
1	B	328	LYS
1	B	333	GLN
1	B	344	ASP
1	B	353	ARG
1	B	362	LEU
1	B	386	ARG
1	B	390	PRO
1	B	392	TYR

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Mol	Chain	Res	Type
1	B	398	HIS
1	B	408	ASP
1	B	424	ARG
1	B	434	ARG
2	C	989	ARG
2	D	991	GLU
2	D	992	ARG
2	F	979	GLN
2	F	982	ILE
2	F	983	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	124	ASN
1	A	167	GLN
1	A	187	ASN
1	A	194	HIS
1	A	246	ASN
1	A	249	GLN
1	A	287	ASN
1	A	296	ASN
1	A	333	GLN
1	A	421	HIS
1	A	425	GLN
1	B	87	ASN
1	B	187	ASN
1	B	246	ASN
1	B	287	ASN
1	B	333	GLN
1	B	425	GLN
2	G	974	GLN
2	G	979	GLN
2	G	988	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	1001	2	7,8,9	0.41	0	5,10,12	1.11	0
2	HYP	C	965	2	7,8,9	0.44	0	5,10,12	1.15	0
2	HYP	C	968	2	7,8,9	0.44	0	5,10,12	1.05	0
2	HYP	C	971	2	7,8,9	0.47	0	5,10,12	1.49	1 (20%)
2	HYP	C	986	2	7,8,9	0.45	0	5,10,12	1.26	1 (20%)
2	HYP	C	995	2	7,8,9	0.52	0	5,10,12	1.12	0
2	HYP	C	998	2	7,8,9	0.41	0	5,10,12	1.08	0
2	HYP	D	965	2	7,8,9	0.42	0	5,10,12	1.05	0
2	HYP	D	968	2	7,8,9	0.44	0	5,10,12	1.21	0
2	HYP	D	971	2	7,8,9	0.45	0	5,10,12	1.19	0
2	HYP	D	986	2	7,8,9	0.45	0	5,10,12	0.96	0
2	HYP	D	995	2	7,8,9	0.48	0	5,10,12	1.28	1 (20%)
2	HYP	D	998	2	7,8,9	0.40	0	5,10,12	1.17	0
2	HYP	E	965	2	7,8,9	0.37	0	5,10,12	1.14	0
2	HYP	E	968	2	7,8,9	0.45	0	5,10,12	1.32	1 (20%)
2	HYP	E	971	2	7,8,9	0.42	0	5,10,12	1.03	0
2	HYP	E	986	2	7,8,9	0.45	0	5,10,12	1.49	1 (20%)
2	HYP	E	995	2	7,8,9	0.38	0	5,10,12	1.08	0
2	HYP	F	965	2	7,8,9	0.43	0	5,10,12	1.19	0
2	HYP	F	968	2	7,8,9	0.55	0	5,10,12	1.35	0
2	HYP	F	971	2	7,8,9	0.50	0	5,10,12	1.23	0
2	HYP	F	986	2	7,8,9	0.57	0	5,10,12	1.62	1 (20%)
2	HYP	F	995	2	7,8,9	0.45	0	5,10,12	0.97	0
2	HYP	F	998	2	7,8,9	0.38	0	5,10,12	1.04	0
2	HYP	G	965	2	7,8,9	0.50	0	5,10,12	1.20	0
2	HYP	G	968	2	7,8,9	0.43	0	5,10,12	1.10	0
2	HYP	G	971	2	7,8,9	0.42	0	5,10,12	1.05	0
2	HYP	G	986	2	7,8,9	0.51	0	5,10,12	0.94	0
2	HYP	G	995	2	7,8,9	0.46	0	5,10,12	0.94	0
2	HYP	G	998	2	7,8,9	0.42	0	5,10,12	1.20	0
2	HYP	H	965	2	7,8,9	0.37	0	5,10,12	0.99	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HYP	H	968	2	7,8,9	0.52	0	5,10,12	1.40	1 (20%)
2	HYP	H	971	2	7,8,9	0.63	0	5,10,12	1.28	0
2	HYP	H	986	2	7,8,9	0.55	0	5,10,12	1.61	2 (40%)
2	HYP	H	995	2	7,8,9	0.47	0	5,10,12	1.00	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	1001	2	-	0/0/11/13	0/1/1/1
2	HYP	C	965	2	-	0/0/11/13	0/1/1/1
2	HYP	C	968	2	-	0/0/11/13	0/1/1/1
2	HYP	C	971	2	-	0/0/11/13	0/1/1/1
2	HYP	C	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	C	998	2	-	0/0/11/13	0/1/1/1
2	HYP	D	965	2	-	0/0/11/13	0/1/1/1
2	HYP	D	968	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	986	2	-	0/0/11/13	0/1/1/1
2	HYP	D	995	2	-	0/0/11/13	0/1/1/1
2	HYP	D	998	2	-	0/0/11/13	0/1/1/1
2	HYP	E	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	E	971	2	-	0/0/11/13	0/1/1/1
2	HYP	E	986	2	-	0/0/11/13	0/1/1/1
2	HYP	E	995	2	-	0/0/11/13	0/1/1/1
2	HYP	F	965	2	-	0/0/11/13	0/1/1/1
2	HYP	F	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	F	986	2	-	0/0/11/13	0/1/1/1
2	HYP	F	995	2	-	0/0/11/13	0/1/1/1
2	HYP	F	998	2	-	0/0/11/13	0/1/1/1
2	HYP	G	965	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	971	2	-	0/0/11/13	0/1/1/1
2	HYP	G	986	2	-	0/0/11/13	0/1/1/1
2	HYP	G	995	2	-	0/0/11/13	0/1/1/1
2	HYP	G	998	2	-	0/0/11/13	0/1/1/1
2	HYP	H	965	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	H	968	2	-	0/0/11/13	0/1/1/1
2	HYP	H	971	2	-	0/0/11/13	0/1/1/1
2	HYP	H	986	2	-	0/0/11/13	0/1/1/1
2	HYP	H	995	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	986	HYP	CB-CG-CD	-2.70	99.80	103.14
2	H	986	HYP	CB-CG-CD	-2.61	99.91	103.14
2	E	986	HYP	CB-CG-CD	-2.41	100.16	103.14
2	H	968	HYP	CB-CG-CD	-2.30	100.29	103.14
2	E	968	HYP	O-C-CA	-2.13	119.81	125.44
2	D	995	HYP	CB-CG-CD	-2.13	100.50	103.14
2	C	986	HYP	O-C-CA	-2.07	119.96	125.44
2	H	986	HYP	O-C-CA	-2.06	119.99	125.44
2	C	971	HYP	CB-CG-CD	-2.03	100.62	103.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 30 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	971	HYP	4	0
2	H	995	HYP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/367 (100%)	-0.56	0 <span>100</span> <span>100</span>	11, 33, 54, 69	0
1	B	367/367 (100%)	-0.66	0 <span>100</span> <span>100</span>	9, 28, 51, 61	0
2	C	32/40 (80%)	-0.02	2 (6%) <span>23</span> <span>9</span>	21, 51, 92, 95	0
2	D	30/40 (75%)	-0.20	1 (3%) <span>50</span> <span>22</span>	25, 38, 77, 81	0
2	E	28/40 (70%)	-0.40	0 <span>100</span> <span>100</span>	24, 44, 68, 69	0
2	F	30/40 (75%)	-0.21	1 (3%) <span>50</span> <span>22</span>	22, 42, 81, 87	0
2	G	30/40 (75%)	-0.40	0 <span>100</span> <span>100</span>	21, 36, 65, 77	0
2	H	28/40 (70%)	-0.47	0 <span>100</span> <span>100</span>	13, 38, 60, 62	0
All	All	912/974 (93%)	-0.54	4 (0%) <span>93</span> <span>80</span>	9, 32, 60, 95	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	963	GLY	2.9
2	C	963	GLY	2.7
2	C	964	PRO	2.3
2	D	963	GLY	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HYP	D	968	8/9	0.93	0.24	-	57,61,62,62	0
2	HYP	C	971	8/9	0.94	0.22	-	44,47,48,49	0
2	HYP	C	968	8/9	0.85	0.23	-	69,71,71,72	0
2	HYP	H	968	8/9	0.95	0.21	-	50,51,52,53	0
2	HYP	E	965	8/9	0.90	0.20	-	61,64,65,65	0
2	HYP	G	998	8/9	0.84	0.26	-	78,80,80,80	0
2	HYP	G	995	8/9	0.94	0.16	-	62,63,66,66	0
2	HYP	G	986	8/9	0.95	0.13	-	33,33,34,36	0
2	HYP	F	968	8/9	0.90	0.22	-	69,72,73,74	0
2	HYP	C	986	8/9	0.96	0.12	-	34,35,36,37	0
2	HYP	G	971	8/9	0.94	0.21	-	40,43,44,44	0
2	HYP	E	971	8/9	0.95	0.16	-	43,45,47,47	0
2	HYP	F	995	8/9	0.89	0.17	-	65,67,68,69	0
2	HYP	H	971	8/9	0.98	0.13	-	34,35,35,36	0
2	HYP	E	968	8/9	0.92	0.24	-	60,61,62,63	0
2	HYP	H	995	8/9	0.88	0.29	-	62,62,63,64	0
2	HYP	G	968	8/9	0.94	0.15	-	51,52,53,53	0
2	HYP	F	986	8/9	0.92	0.18	-	31,32,34,34	0
2	HYP	C	1001	8/9	0.64	0.30	-	94,95,95,96	0
2	HYP	F	998	8/9	0.79	0.33	-	72,74,75,75	0
2	HYP	C	965	8/9	0.83	0.29	-	87,89,90,90	0
2	HYP	F	965	8/9	0.91	0.27	-	83,85,85,85	0
2	HYP	D	995	8/9	0.90	0.19	-	68,69,70,71	0
2	HYP	D	971	8/9	0.95	0.23	-	41,43,43,43	0
2	HYP	E	995	8/9	0.90	0.33	-	70,72,73,74	0
2	HYP	C	998	8/9	0.85	0.27	-	88,89,90,90	0
2	HYP	E	986	8/9	0.95	0.21	-	44,44,45,47	0
2	HYP	D	986	8/9	0.93	0.18	-	30,31,31,34	0
2	HYP	H	965	8/9	0.87	0.21	-	60,62,63,63	0
2	HYP	D	998	8/9	0.82	0.32	-	84,84,85,86	0
2	HYP	H	986	8/9	0.97	0.16	-	32,34,36,36	0
2	HYP	D	965	8/9	0.65	0.35	-	75,77,78,78	0
2	HYP	G	965	8/9	0.90	0.20	-	58,61,61,62	0
2	HYP	F	971	8/9	0.96	0.20	-	51,54,55,56	0
2	HYP	C	995	8/9	0.92	0.18	-	73,74,78,79	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	B	1103	1/1	0.69	0.15	0.83	95,95,95,95	0
3	CA	B	1101	1/1	0.80	0.16	-0.09	70,70,70,70	0
3	CA	B	1104	1/1	0.99	0.09	-1.51	16,16,16,16	0
3	CA	A	1103	1/1	0.94	0.08	-1.70	63,63,63,63	0
3	CA	A	1104	1/1	0.96	0.08	-1.91	25,25,25,25	0
4	ZN	B	1201	1/1	1.00	0.08	-2.51	25,25,25,25	0
4	ZN	A	1201	1/1	0.99	0.06	-3.29	35,35,35,35	0
3	CA	A	1102	1/1	0.96	0.04	-3.67	40,40,40,40	0
3	CA	B	1102	1/1	0.96	0.06	-3.88	31,31,31,31	0
4	ZN	B	1202	1/1	0.99	0.14	-	20,20,20,20	0
3	CA	A	1101	1/1	0.59	0.11	-	68,68,68,68	0
4	ZN	A	1202	1/1	0.98	0.15	-	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.