



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:43 AM UTC

PDB ID : 3VI2 / pdb_00003vi2
Title : Crystal Structure Analysis of Plasmodium falciparum OMP Decarboxylase in complex with inhibitor HMOA
Authors : Takashima, Y.; Mizohata, E.; Krungkrai, S.R.; Matsumura, H.; Krungkrai, J.; Horii, T.; Inoue, T.
Deposited on : 2011-09-16
Resolution : 2.10 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

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

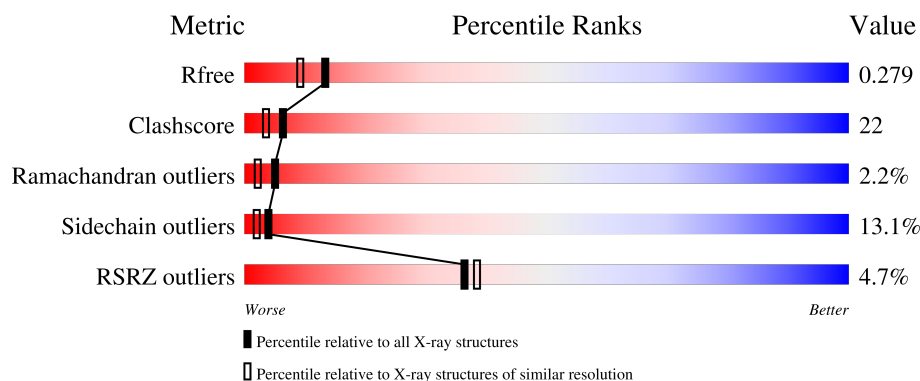
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	323	5% 54% 33% 10% ..
1	B	323	4% 62% 29% 8% .

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	HMZ	A	500	-	-	X	-
2	HMZ	B	600	-	-	X	-

2 Entry composition [i](#)

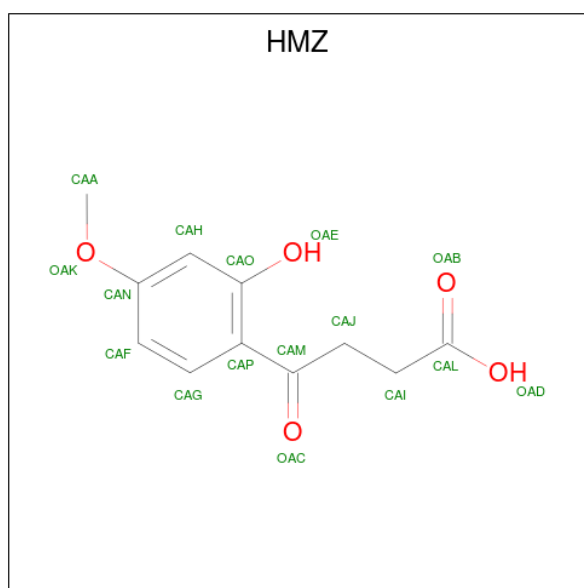
There are 4 unique types of molecules in this entry. The entry contains 5385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2621	1692	422	491	16			
1	B	318	Total	C	N	O	S	0	0	0
			2621	1692	422	491	16			

- Molecule 2 is 4-(2-hydroxy-4-methoxyphenyl)-4-oxobutanoic acid (CCD ID: HMZ) (formula: $C_{11}H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	11	5		
2	B	1	Total	C	O	0	0
			16	11	5		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	2	Total 2	Na 2	0	0

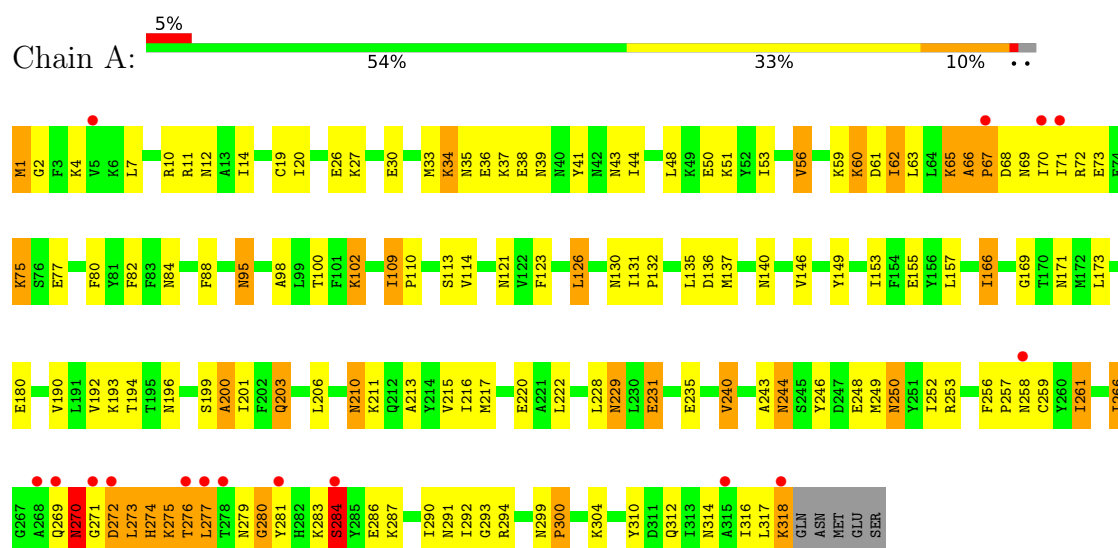
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total 63	O 63	0	0
4	B	45	Total 45	O 45	0	0

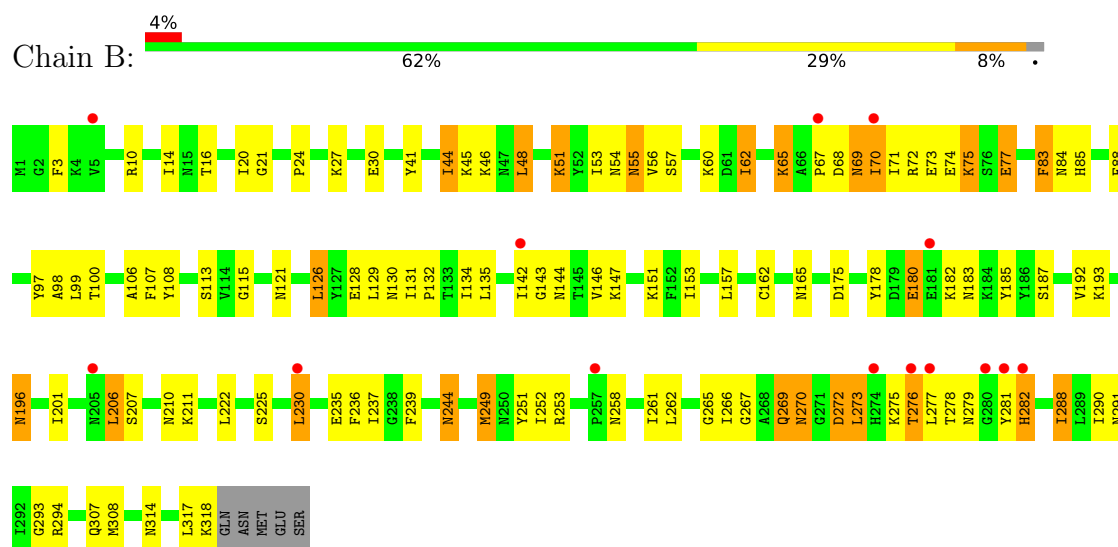
3 Residue-property plots [i](#)

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: Orotidine 5'-phosphate decarboxylase



• Molecule 1: Orotidine 5'-phosphate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	201.97Å 201.97Å 44.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.50 – 2.10 39.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.50-2.10) 95.0 (39.50-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.284 0.213 , 0.279	Depositor DCC
R_{free} test set	1864 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: NA, HMZ

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	1.19	9/2677 (0.3%)	1.31	16/3609 (0.4%)
1	B	1.01	2/2677 (0.1%)	1.14	2/3609 (0.1%)
All	All	1.10	11/5354 (0.2%)	1.22	18/7218 (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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	ILE	CA-CB	6.66	1.60	1.54
1	A	215	VAL	CA-CB	6.25	1.61	1.54
1	A	131	ILE	C-O	-5.83	1.18	1.24
1	A	114	VAL	CA-CB	5.81	1.60	1.54
1	A	109	ILE	CA-C	5.67	1.58	1.52
1	A	266	ILE	CA-CB	5.51	1.61	1.54
1	B	107	PHE	N-CA	5.37	1.53	1.46
1	A	240	VAL	CA-CB	5.32	1.60	1.54
1	A	126	LEU	CA-C	5.28	1.59	1.52
1	A	123	PHE	N-CA	5.13	1.52	1.46
1	A	292	ILE	CA-CB	5.09	1.60	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	LYS	N-CA-C	-10.58	101.12	114.56
1	A	66	ALA	CA-C-N	7.02	128.61	119.84
1	A	66	ALA	C-N-CA	7.02	128.61	119.84
1	A	69	ASN	N-CA-C	-6.81	105.59	114.04
1	A	274	HIS	N-CA-C	-6.52	104.10	111.14
1	A	137	MET	N-CA-C	-6.16	106.98	114.75
1	A	280	GLY	N-CA-C	-6.14	98.63	113.18
1	A	14	ILE	N-CA-C	5.99	119.52	113.47
1	B	83	PHE	N-CA-C	-5.86	104.80	111.07
1	A	200	ALA	N-CA-C	5.65	118.38	111.82
1	A	130	ASN	CA-C-N	-5.51	117.36	123.43
1	A	130	ASN	C-N-CA	-5.51	117.36	123.43
1	A	155	GLU	N-CA-C	-5.47	105.66	112.93
1	A	169	GLY	N-CA-C	5.29	117.26	110.96
1	A	271	GLY	N-CA-C	-5.29	102.42	112.27
1	B	230	LEU	N-CA-C	5.25	116.81	111.14
1	A	272	ASP	N-CA-C	5.12	117.79	109.86
1	A	95	ASN	N-CA-C	5.10	117.74	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	ASN	Peptide
1	A	284	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	2621	0	2598	141	0
1	B	2621	0	2598	97	0
2	A	16	0	11	6	0
2	B	16	0	11	13	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	63	0	0	1	0
4	B	45	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5385	0	5218	232	0

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

All (232) 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:100:THR:HG22	1:B:132:PRO:HB2	1.25	1.19
1:B:225:SER:HB2	1:B:230:LEU:HD11	1.18	1.18
1:B:249:MET:HE1	1:B:261:ILE:HD13	1.22	1.16
1:A:246:TYR:HD2	1:A:276:THR:CG2	1.60	1.15
1:A:246:TYR:CD2	1:A:276:THR:HG22	1.80	1.15
1:A:243:ALA:HB1	1:A:277:LEU:HD23	1.31	1.11
1:A:113:SER:HB2	1:B:113:SER:HB2	1.29	1.09
1:B:291:ASN:HD21	2:B:600:HMZ:HAAA	1.00	1.08
1:A:246:TYR:CD2	1:A:276:THR:CG2	2.35	1.07
1:A:36:GLU:HG3	1:A:41:TYR:HA	1.37	1.06
1:A:283:LYS:HD3	1:A:284:SER:H	0.98	1.06
1:B:291:ASN:HD21	2:B:600:HMZ:CAA	1.73	1.00
1:A:259:CYS:SG	1:A:281:TYR:OH	2.20	0.99
1:B:291:ASN:ND2	2:B:600:HMZ:HAAA	1.76	0.98
1:B:244:ASN:H	1:B:244:ASN:HD22	0.99	0.96
1:A:277:LEU:HD12	1:A:277:LEU:H	1.27	0.96
1:A:62:ILE:HD12	1:A:77:GLU:HG2	1.48	0.95
1:A:246:TYR:HD2	1:A:276:THR:HG22	1.17	0.95
1:A:283:LYS:HD3	1:A:284:SER:N	1.83	0.92
1:A:274:HIS:O	1:A:276:THR:N	2.03	0.92
1:B:75:LYS:HA	1:B:75:LYS:HE2	1.55	0.88
1:B:273:LEU:O	1:B:277:LEU:HD21	1.78	0.84
1:B:55:ASN:HB3	1:B:128:GLU:HG3	1.60	0.84
1:A:249:MET:HG3	1:A:281:TYR:HB2	1.59	0.82
1:A:246:TYR:CD2	1:A:276:THR:HG21	2.12	0.82
1:B:294:ARG:NH2	2:B:600:HMZ:HAJA	1.94	0.82
1:A:291:ASN:HD21	2:A:500:HMZ:HAAB	1.45	0.81
1:B:100:THR:HG22	1:B:132:PRO:CB	2.09	0.81
1:A:293:GLY:HA3	2:A:500:HMZ:OAK	1.79	0.81
1:B:147:LYS:HG2	1:B:175:ASP:HB3	1.61	0.81
1:A:253:ARG:CZ	1:A:281:TYR:CD1	2.64	0.80
1:B:51:LYS:H	1:B:51:LYS:HD3	1.48	0.79
1:B:244:ASN:HD22	1:B:244:ASN:N	1.79	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:HA3	2:B:600:HMZ:HAH	1.66	0.77
1:A:253:ARG:CZ	1:A:281:TYR:CE1	2.68	0.76
1:A:253:ARG:HB2	1:A:281:TYR:CG	2.20	0.76
1:A:166:ILE:HD13	1:A:190:VAL:HG11	1.66	0.75
1:A:248:GLU:O	1:A:252:ILE:HD12	1.86	0.75
1:A:277:LEU:HD12	1:A:277:LEU:N	2.02	0.75
1:A:269:GLN:HG2	1:A:270:ASN:N	2.01	0.74
1:A:283:LYS:CD	1:A:284:SER:H	1.89	0.74
1:B:265:GLY:O	1:B:269:GLN:HB3	1.86	0.74
1:B:68:ASP:O	1:B:72:ARG:HB3	1.87	0.74
1:A:243:ALA:HB1	1:A:277:LEU:CD2	2.15	0.72
1:A:253:ARG:HG2	1:A:281:TYR:HA	1.70	0.72
1:B:293:GLY:CA	2:B:600:HMZ:HAH	2.18	0.72
1:A:210:ASN:N	1:A:210:ASN:HD22	1.88	0.71
1:B:249:MET:SD	1:B:281:TYR:OH	2.47	0.71
1:B:84:ASN:HD21	1:B:121:ASN:HD22	1.38	0.70
1:A:246:TYR:CB	1:A:276:THR:HG21	2.22	0.70
1:A:277:LEU:H	1:A:277:LEU:CD1	2.04	0.70
1:B:21:GLY:HA3	2:B:600:HMZ:CAA	2.23	0.69
1:A:166:ILE:HD13	1:A:190:VAL:CG1	2.23	0.69
1:A:291:ASN:HD21	2:A:500:HMZ:CAA	2.07	0.68
1:A:166:ILE:CD1	1:A:190:VAL:CG1	2.72	0.68
1:B:294:ARG:HH21	2:B:600:HMZ:HAJA	1.56	0.67
1:B:244:ASN:H	1:B:244:ASN:ND2	1.79	0.67
1:A:110:PRO:HB2	1:B:151:LYS:HE2	1.76	0.67
1:A:11:ARG:HH21	1:A:12:ASN:HD21	1.41	0.67
1:B:272:ASP:HB2	1:B:275:LYS:HB2	1.77	0.67
1:B:281:TYR:N	1:B:281:TYR:CD1	2.61	0.66
1:A:273:LEU:O	1:A:277:LEU:HD13	1.96	0.66
1:B:56:VAL:HG11	1:B:88:PHE:HZ	1.59	0.66
1:A:253:ARG:NH2	1:A:281:TYR:CD1	2.65	0.65
1:A:246:TYR:HB3	1:A:276:THR:HG21	1.79	0.64
1:B:100:THR:CG2	1:B:132:PRO:HB2	2.17	0.64
1:A:20:ILE:HD12	1:A:98:ALA:HB2	1.77	0.64
1:A:1:MET:HG2	1:A:2:GLY:H	1.63	0.64
1:A:140:ASN:ND2	1:B:165:ASN:HD22	1.95	0.64
1:B:135:LEU:HD23	1:B:153:ILE:HG12	1.78	0.63
1:B:65:LYS:HD3	1:B:69:ASN:HB3	1.80	0.63
1:A:253:ARG:CG	1:A:281:TYR:HA	2.29	0.62
1:A:266:ILE:HD11	1:A:277:LEU:CD2	2.30	0.62
1:A:272:ASP:O	1:A:277:LEU:HD11	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD23	1:B:278:THR:H	1.66	0.61
1:A:273:LEU:C	1:A:277:LEU:HD13	2.24	0.61
1:A:284:SER:O	1:A:287:LYS:HG3	2.01	0.61
1:B:10:ARG:HG2	1:B:99:LEU:HD12	1.82	0.61
1:B:71:ILE:HG12	1:B:75:LYS:HD2	1.84	0.60
1:A:4:LYS:NZ	1:A:231:GLU:HG3	2.16	0.60
1:A:253:ARG:CB	1:A:281:TYR:HA	2.31	0.60
1:A:26:GLU:O	1:A:30:GLU:HG2	2.01	0.60
1:A:261:ILE:CG2	1:A:281:TYR:CE1	2.84	0.59
1:B:126:LEU:HD12	1:B:131:ILE:HD12	1.83	0.59
1:B:230:LEU:HD13	1:B:236:PHE:HA	1.85	0.59
1:A:291:ASN:ND2	2:A:500:HMZ:HAAB	2.14	0.59
1:B:178:TYR:CE2	1:B:180:GLU:HG2	2.37	0.59
1:A:166:ILE:CD1	1:A:190:VAL:HG11	2.33	0.59
1:A:102:LYS:HE2	1:A:136:ASP:OD2	2.02	0.59
1:A:261:ILE:HG21	1:A:281:TYR:CE1	2.37	0.58
1:A:36:GLU:C	1:A:38:GLU:H	2.11	0.58
1:A:166:ILE:CD1	1:A:190:VAL:HG12	2.33	0.58
1:B:84:ASN:ND2	1:B:121:ASN:HD22	2.02	0.58
1:B:53:ILE:HG13	1:B:88:PHE:CE2	2.39	0.58
1:A:56:VAL:O	1:A:60:LYS:HG3	2.04	0.58
1:A:253:ARG:NH2	1:A:281:TYR:HD1	2.01	0.57
1:A:274:HIS:C	1:A:276:THR:H	2.11	0.57
1:B:267:GLY:H	1:B:270:ASN:HA	1.69	0.57
1:B:225:SER:HB3	1:B:237:ILE:HB	1.87	0.57
1:A:100:THR:HG22	1:A:132:PRO:HB2	1.86	0.57
1:B:69:ASN:HD22	1:B:69:ASN:H	1.53	0.57
1:A:244:ASN:HD22	1:A:244:ASN:H	1.52	0.56
1:A:280:GLY:O	1:A:281:TYR:CB	2.53	0.56
1:A:261:ILE:HG21	1:A:281:TYR:CD1	2.40	0.56
1:B:21:GLY:HA3	2:B:600:HMZ:HAA	1.86	0.56
1:B:21:GLY:HA3	2:B:600:HMZ:HAAB	1.87	0.56
1:A:19:CYS:O	1:A:291:ASN:HA	2.05	0.56
1:B:135:LEU:O	1:B:162:CYS:HA	2.05	0.56
1:B:196:ASN:H	1:B:196:ASN:ND2	2.04	0.56
1:A:249:MET:CG	1:A:281:TYR:HB2	2.35	0.55
1:A:44:ILE:O	1:A:48:LEU:HG	2.08	0.54
1:B:54:ASN:ND2	1:B:60:LYS:NZ	2.55	0.54
1:A:246:TYR:CG	1:A:276:THR:HG21	2.43	0.54
1:A:135:LEU:HD23	1:A:153:ILE:HG12	1.90	0.53
1:B:24:PRO:HG2	1:B:83:PHE:HE1	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:SER:O	1:A:203:GLN:HB2	2.09	0.53
1:B:143:GLY:O	1:B:147:LYS:HG3	2.09	0.53
1:A:210:ASN:N	1:A:210:ASN:ND2	2.53	0.53
1:A:216:ILE:HG23	1:A:217:MET:N	2.23	0.52
1:A:2:GLY:HA2	1:A:235:GLU:OE2	2.09	0.52
1:A:253:ARG:NH1	1:A:281:TYR:CE1	2.77	0.52
1:A:269:GLN:CG	1:A:270:ASN:N	2.72	0.52
1:B:273:LEU:O	1:B:278:THR:HG22	2.09	0.51
1:B:41:TYR:HB2	1:B:45:LYS:HE3	1.92	0.51
1:B:97:TYR:CZ	1:B:307:GLN:HB2	2.45	0.51
1:A:84:ASN:ND2	1:A:121:ASN:HD22	2.09	0.51
1:A:194:THR:H	1:A:203:GLN:NE2	2.08	0.51
1:A:316:ILE:C	1:A:318:LYS:H	2.19	0.51
1:B:253:ARG:HH21	1:B:261:ILE:HD12	1.75	0.51
1:A:1:MET:SD	1:A:1:MET:N	2.64	0.51
1:A:310:TYR:CE2	1:A:314:ASN:ND2	2.79	0.51
1:B:196:ASN:H	1:B:196:ASN:HD22	1.58	0.51
1:B:207:SER:HB2	1:B:211:LYS:O	2.11	0.50
1:A:277:LEU:O	1:A:280:GLY:O	2.30	0.50
1:A:56:VAL:HG11	1:A:88:PHE:HZ	1.76	0.50
1:B:129:LEU:O	1:B:130:ASN:C	2.55	0.50
1:A:63:LEU:HD13	1:A:80:PHE:CE2	2.47	0.50
1:A:63:LEU:HD11	1:A:84:ASN:HB3	1.93	0.50
1:B:62:ILE:HG12	1:B:77:GLU:HG2	1.94	0.50
1:B:275:LYS:C	1:B:277:LEU:H	2.19	0.49
1:A:253:ARG:NE	1:A:281:TYR:CD1	2.80	0.49
1:A:36:GLU:CG	1:A:41:TYR:HA	2.26	0.49
1:B:48:LEU:HD13	1:B:85:HIS:HE1	1.76	0.49
1:B:75:LYS:HE2	1:B:75:LYS:CA	2.27	0.49
1:A:194:THR:H	1:A:203:GLN:HE22	1.60	0.49
1:A:62:ILE:HA	1:A:65:LYS:HD3	1.94	0.49
1:B:135:LEU:CD2	1:B:153:ILE:HG12	2.42	0.49
1:A:246:TYR:HD2	1:A:276:THR:HG21	1.53	0.49
1:A:293:GLY:HA3	2:A:500:HMZ:CAN	2.42	0.49
1:A:35:ASN:O	1:A:39:ASN:OD1	2.31	0.49
1:A:36:GLU:OE2	1:A:43:ASN:N	2.46	0.48
1:B:273:LEU:C	1:B:277:LEU:HD21	2.37	0.48
1:A:250:ASN:ND2	1:A:280:GLY:CA	2.76	0.48
1:A:62:ILE:O	1:A:65:LYS:HB2	2.14	0.48
1:A:274:HIS:HD2	1:A:316:ILE:HG23	1.78	0.48
1:B:249:MET:HB3	1:B:281:TYR:OH	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:SER:CB	1:B:211:LYS:O	2.62	0.48
1:B:53:ILE:HG13	1:B:88:PHE:HE2	1.79	0.48
1:A:253:ARG:HB2	1:A:281:TYR:CD2	2.48	0.48
1:A:276:THR:O	1:A:280:GLY:N	2.40	0.48
1:B:251:TYR:HD2	1:B:252:ILE:HD12	1.79	0.48
1:A:299:ASN:HA	1:A:300:PRO:HD2	1.67	0.47
1:B:56:VAL:HG11	1:B:88:PHE:CZ	2.46	0.47
1:B:187:SER:OG	1:B:235:GLU:OE1	2.25	0.47
1:A:274:HIS:C	1:A:276:THR:N	2.67	0.47
1:B:293:GLY:N	2:B:600:HMZ:HAH	2.27	0.47
1:A:253:ARG:NH2	1:A:281:TYR:CE1	2.82	0.47
1:A:7:LEU:HB3	1:A:286:GLU:HG3	1.96	0.47
1:A:166:ILE:HD11	1:A:173:LEU:HD21	1.97	0.47
1:A:266:ILE:HD11	1:A:277:LEU:HD21	1.96	0.47
1:B:70:ILE:HG23	1:B:71:ILE:H	1.79	0.47
1:B:54:ASN:ND2	1:B:60:LYS:HZ1	2.12	0.47
1:B:276:THR:O	1:B:276:THR:OG1	2.31	0.46
1:B:288:ILE:CD1	1:B:290:ILE:HD11	2.46	0.46
1:A:200:ALA:O	1:A:201:ILE:C	2.58	0.46
1:A:149:TYR:CZ	1:B:106:ALA:HB2	2.51	0.46
1:B:73:GLU:O	1:B:75:LYS:N	2.49	0.46
1:A:246:TYR:CE2	1:A:276:THR:HG22	2.45	0.46
1:A:283:LYS:HD2	1:A:287:LYS:HD2	1.98	0.46
1:B:143:GLY:O	1:B:144:ASN:C	2.57	0.46
1:B:277:LEU:HD23	1:B:277:LEU:H	1.80	0.46
1:A:250:ASN:ND2	1:A:280:GLY:HA3	2.31	0.45
1:B:269:GLN:HB2	2:B:600:HMZ:CAL	2.46	0.45
1:B:16:THR:CB	1:B:314:ASN:HD21	2.29	0.45
1:A:273:LEU:HD12	1:A:312:GLN:HE21	1.81	0.45
1:A:60:LYS:HE3	1:A:60:LYS:HB3	1.64	0.45
1:A:243:ALA:CB	1:A:277:LEU:HD23	2.23	0.45
1:B:281:TYR:O	1:B:282:HIS:CG	2.70	0.45
1:A:216:ILE:HG21	1:B:206:LEU:HD11	1.98	0.45
1:A:166:ILE:O	1:A:166:ILE:CG2	2.64	0.45
1:A:66:ALA:HA	1:A:67:PRO:HD2	1.79	0.44
1:A:4:LYS:HZ2	1:A:231:GLU:HG3	1.80	0.44
1:A:51:LYS:NZ	4:A:349:HOH:O	2.48	0.44
1:A:193:LYS:HB3	1:A:193:LYS:HE3	1.67	0.44
1:A:250:ASN:ND2	1:A:280:GLY:HA2	2.32	0.44
1:A:50:GLU:O	1:A:53:ILE:HG22	2.17	0.44
1:A:59:LYS:HB3	1:A:62:ILE:HG13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:O	1:A:65:LYS:HD2	2.17	0.44
1:A:34:LYS:HE2	1:A:38:GLU:HG3	1.98	0.44
1:A:220:GLU:HG2	1:B:201:ILE:CD1	2.48	0.44
1:A:84:ASN:HD21	1:A:121:ASN:HD22	1.65	0.44
1:A:261:ILE:HG22	1:A:287:LYS:O	2.18	0.44
1:A:272:ASP:O	1:A:277:LEU:CD1	2.65	0.44
1:A:192:VAL:HB	1:A:240:VAL:O	2.18	0.43
1:A:196:ASN:O	1:A:199:SER:HB3	2.17	0.43
1:B:128:GLU:C	1:B:130:ASN:H	2.26	0.43
1:A:249:MET:SD	1:A:281:TYR:CD2	3.11	0.43
1:B:3:PHE:HE1	1:B:132:PRO:HB3	1.84	0.43
1:B:44:ILE:HG21	1:B:67:PRO:HG3	1.99	0.43
1:A:4:LYS:HZ1	1:A:231:GLU:HG3	1.84	0.43
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.93	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.81	0.43
1:A:256:PHE:C	1:A:257:PRO:O	2.56	0.43
1:A:10:ARG:HD3	1:A:132:PRO:HD2	2.00	0.43
1:B:153:ILE:HG21	1:B:162:CYS:HB3	2.01	0.42
1:A:249:MET:O	1:A:281:TYR:HD2	2.02	0.42
1:A:252:ILE:HB	1:A:281:TYR:HE2	1.85	0.42
1:B:293:GLY:H	2:B:600:HMZ:HAH	1.84	0.42
1:B:183:ASN:CG	1:B:183:ASN:O	2.62	0.42
1:B:225:SER:HB3	1:B:237:ILE:HD12	2.02	0.41
1:A:196:ASN:ND2	1:A:196:ASN:H	2.18	0.41
1:B:249:MET:SD	1:B:281:TYR:CZ	3.12	0.41
1:A:228:LEU:O	1:A:229:ASN:HB2	2.21	0.41
1:B:20:ILE:HD12	1:B:98:ALA:HB2	2.03	0.41
1:B:108:TYR:O	1:B:115:GLY:HA3	2.20	0.41
1:B:192:VAL:HG21	1:B:239:PHE:HB3	2.03	0.41
1:A:33:MET:HB2	1:A:82:PHE:CG	2.55	0.41
1:A:275:LYS:HD2	1:A:275:LYS:HA	1.78	0.41
1:B:54:ASN:HD21	1:B:60:LYS:NZ	2.18	0.41
1:A:213:ALA:O	1:A:216:ILE:HG22	2.21	0.40
1:A:294:ARG:HD2	2:A:500:HMZ:CAG	2.51	0.40
1:B:55:ASN:HD22	1:B:55:ASN:HA	1.64	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	316/323 (98%)	282 (89%)	25 (8%)	9 (3%)	4	1
1	B	316/323 (98%)	286 (90%)	25 (8%)	5 (2%)	7	4
All	All	632/646 (98%)	568 (90%)	50 (8%)	14 (2%)	5	2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	276	THR
1	B	74	GLU
1	A	37	LYS
1	A	68	ASP
1	A	73	GLU
1	B	70	ILE
1	B	270	ASN
1	B	282	HIS
1	A	67	PRO
1	A	317	LEU
1	B	258	ASN
1	A	300	PRO
1	A	70	ILE

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	290/295 (98%)	253 (87%)	37 (13%)	4	2
1	B	290/295 (98%)	251 (87%)	39 (13%)	4	2
All	All	580/590 (98%)	504 (87%)	76 (13%)	4	2

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	LYS
1	A	34	LYS
1	A	56	VAL
1	A	60	LYS
1	A	62	ILE
1	A	65	LYS
1	A	71	ILE
1	A	72	ARG
1	A	75	LYS
1	A	95	ASN
1	A	102	LYS
1	A	126	LEU
1	A	146	VAL
1	A	157	LEU
1	A	166	ILE
1	A	171	ASN
1	A	180	GLU
1	A	203	GLN
1	A	206	LEU
1	A	210	ASN
1	A	211	LYS
1	A	222	LEU
1	A	229	ASN
1	A	231	GLU
1	A	244	ASN
1	A	250	ASN
1	A	258	ASN
1	A	261	ILE
1	A	270	ASN
1	A	273	LEU
1	A	277	LEU
1	A	279	ASN
1	A	284	SER
1	A	290	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	304	LYS
1	A	318	LYS
1	B	14	ILE
1	B	27	LYS
1	B	30	GLU
1	B	44	ILE
1	B	46	LYS
1	B	48	LEU
1	B	51	LYS
1	B	55	ASN
1	B	57	SER
1	B	62	ILE
1	B	65	LYS
1	B	69	ASN
1	B	75	LYS
1	B	77	GLU
1	B	126	LEU
1	B	134	ILE
1	B	146	VAL
1	B	157	LEU
1	B	180	GLU
1	B	182	LYS
1	B	185	TYR
1	B	193	LYS
1	B	196	ASN
1	B	206	LEU
1	B	210	ASN
1	B	222	LEU
1	B	244	ASN
1	B	249	MET
1	B	262	LEU
1	B	266	ILE
1	B	269	GLN
1	B	272	ASP
1	B	273	LEU
1	B	276	THR
1	B	279	ASN
1	B	288	ILE
1	B	308	MET
1	B	317	LEU
1	B	318	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	31	ASN
1	A	35	ASN
1	A	39	ASN
1	A	55	ASN
1	A	84	ASN
1	A	92	ASN
1	A	95	ASN
1	A	140	ASN
1	A	148	ASN
1	A	196	ASN
1	A	203	GLN
1	A	210	ASN
1	A	219	GLN
1	A	244	ASN
1	A	250	ASN
1	A	274	HIS
1	A	282	HIS
1	A	291	ASN
1	A	303	GLN
1	A	312	GLN
1	B	12	ASN
1	B	35	ASN
1	B	39	ASN
1	B	40	ASN
1	B	54	ASN
1	B	55	ASN
1	B	69	ASN
1	B	84	ASN
1	B	92	ASN
1	B	95	ASN
1	B	196	ASN
1	B	203	GLN
1	B	210	ASN
1	B	219	GLN
1	B	244	ASN
1	B	269	GLN
1	B	279	ASN
1	B	291	ASN
1	B	303	GLN
1	B	314	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	HMZ	B	600	-	16,16,16	1.89	4 (25%)	21,21,21	1.59	3 (14%)
2	HMZ	A	500	-	16,16,16	1.77	3 (18%)	21,21,21	1.99	3 (14%)

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	HMZ	B	600	-	-	7/11/11/11	0/1/1/1
2	HMZ	A	500	-	-	8/11/11/11	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HMZ	CAP-CAM	4.35	1.56	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HMZ	CAJ-CAM	3.95	1.57	1.51
2	B	600	HMZ	CAP-CAM	3.85	1.55	1.48
2	A	500	HMZ	OAK-CAN	3.49	1.44	1.37
2	B	600	HMZ	CAI-CAL	2.78	1.57	1.50
2	B	600	HMZ	CAP-CAO	-2.56	1.37	1.40
2	A	500	HMZ	CAJ-CAM	2.34	1.54	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HMZ	CAO-CAP-CAM	7.03	125.40	120.09
2	B	600	HMZ	CAI-CAJ-CAM	4.39	117.97	112.60
2	B	600	HMZ	CAO-CAP-CAM	4.10	123.18	120.09
2	A	500	HMZ	CAO-CAH-CAN	3.58	123.61	119.50
2	B	600	HMZ	CAO-CAH-CAN	2.23	122.07	119.50
2	A	500	HMZ	OAB-CAL-CAI	-2.21	116.09	123.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HMZ	OAC-CAM-CAP-CAO
2	A	500	HMZ	CAJ-CAM-CAP-CAO
2	A	500	HMZ	CAF-CAN-OAK-CAA
2	B	600	HMZ	CAF-CAN-OAK-CAA
2	A	500	HMZ	CAH-CAN-OAK-CAA
2	B	600	HMZ	CAH-CAN-OAK-CAA
2	A	500	HMZ	CAI-CAJ-CAM-CAP
2	A	500	HMZ	CAI-CAJ-CAM-OAC
2	B	600	HMZ	OAC-CAM-CAP-CAO
2	B	600	HMZ	CAJ-CAM-CAP-CAO
2	B	600	HMZ	CAI-CAJ-CAM-OAC
2	A	500	HMZ	OAC-CAM-CAP-CAG
2	B	600	HMZ	CAI-CAJ-CAM-CAP
2	B	600	HMZ	CAJ-CAM-CAP-CAG
2	A	500	HMZ	CAL-CAI-CAJ-CAM

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	HMZ	13	0
2	A	500	HMZ	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/323 (98%)	0.30	16 (5%) 34 36	30, 56, 88, 118	0
1	B	318/323 (98%)	0.44	14 (4%) 39 41	33, 63, 98, 111	0
All	All	636/646 (98%)	0.37	30 (4%) 36 38	30, 59, 94, 118	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	ILE	4.0
1	B	230	LEU	3.9
1	A	281	TYR	3.8
1	A	284	SER	3.7
1	A	258	ASN	3.3
1	B	276	THR	3.3
1	A	271	GLY	3.3
1	A	70	ILE	3.3
1	A	272	ASP	3.2
1	B	5	VAL	3.2
1	B	277	LEU	3.2
1	A	315	ALA	3.0
1	A	276	THR	2.8
1	A	277	LEU	2.6
1	B	281	TYR	2.5
1	A	268	ALA	2.5
1	B	142	ILE	2.3
1	B	274	HIS	2.3
1	B	67	PRO	2.3
1	B	181	GLU	2.3
1	B	282	HIS	2.3
1	A	278	THR	2.3
1	B	205	ASN	2.2
1	B	70	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	257	PRO	2.2
1	A	5	VAL	2.1
1	B	280	GLY	2.1
1	A	67	PRO	2.1
1	A	269	GLN	2.1
1	A	318	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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
2	HMZ	A	500	16/16	0.76	0.17	60,77,84,85	0
2	HMZ	B	600	16/16	0.77	0.17	64,75,84,86	0
3	NA	B	325	1/1	0.78	0.14	95,95,95,95	0
3	NA	A	324	1/1	0.80	0.17	93,93,93,93	0
3	NA	B	324	1/1	0.86	0.15	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.