



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:55 PM GMT

PDB ID : 3VI2
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

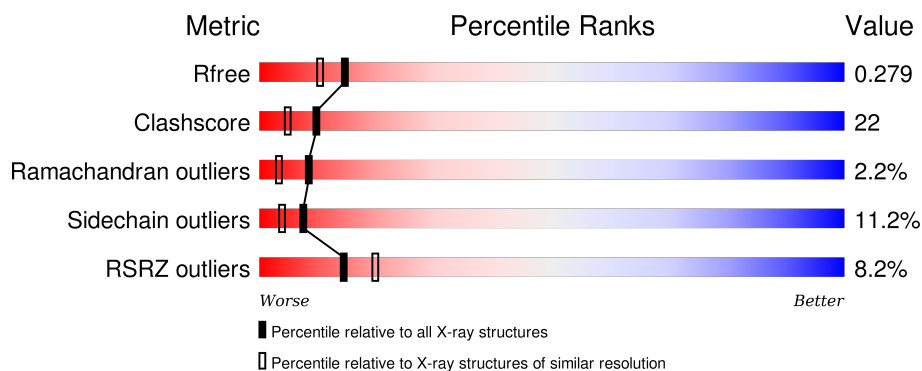
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	323	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	323	<div> <div>11%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>6%</div> <div>•</div> </div> </div>

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	X
2	HMZ	B	600	-	-	X	X

2 Entry composition [i](#)

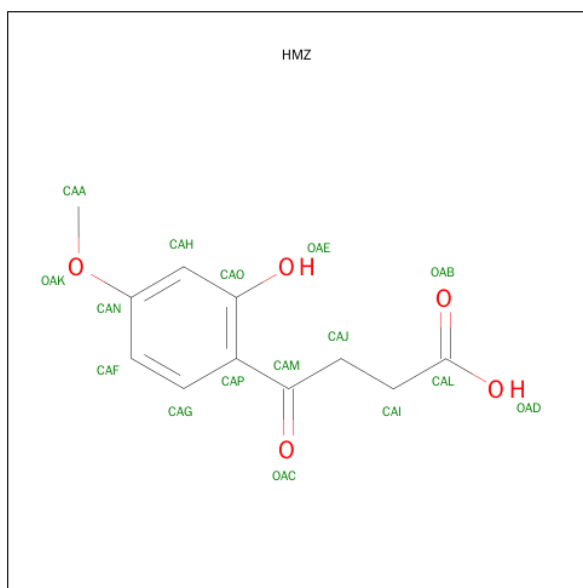
There are 4 unique types of molecules in this entry. The entry contains 5385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: HMZ) (formula: C₁₁H₁₂O₅).



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 (three-letter code: NA) (formula: Na).

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

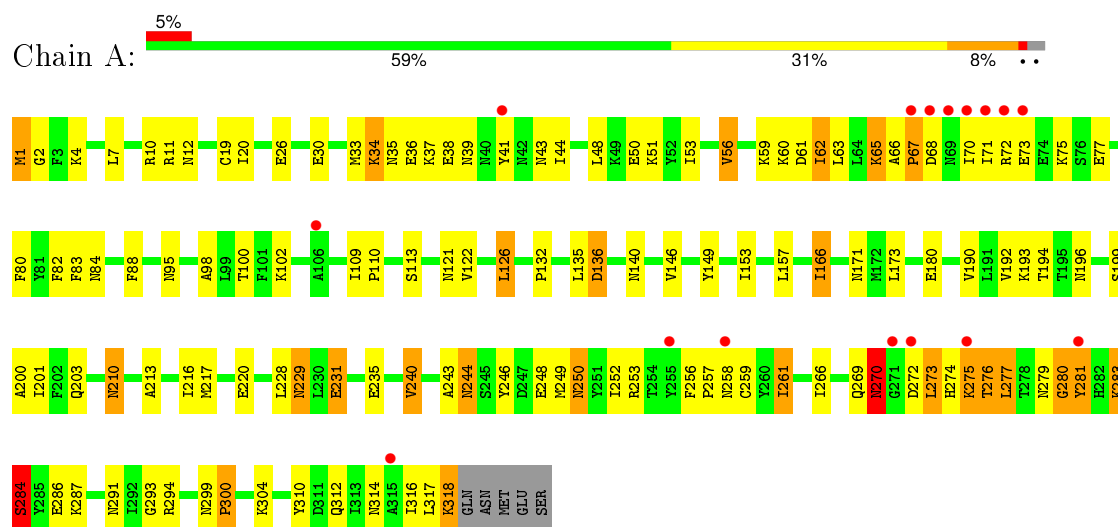
- Molecule 4 is water.

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

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: 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) 95.1 (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 (5.26%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.5	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 37285 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.00	2/2677 (0.1%)	0.93	4/3609 (0.1%)
1	B	0.85	1/2677 (0.0%)	0.84	3/3609 (0.1%)
All	All	0.93	3/5354 (0.1%)	0.89	7/7218 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	CB-CG2	6.69	1.66	1.52
1	B	149	TYR	CD2-CE2	5.81	1.48	1.39
1	A	240	VAL	CB-CG2	5.57	1.64	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	230	LEU	CA-CB-CG	6.47	130.17	115.30
1	A	280	GLY	N-CA-C	-5.79	98.63	113.10
1	A	136	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	23	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	136	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	126	LEU	CB-CG-CD1	5.01	119.52	111.00

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

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	140	0
1	B	2621	0	2598	100	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
All	All	5385	0	5218	234	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 (234) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:B:244:ASN:H	0.99	0.96
1:A:277:LEU:HD12	1:A:277:LEU:H	1.27	0.96
1:A:246:TYR:HD2	1:A:276:THR:HG22	1.17	0.95
1:A:62:ILE:HD12	1:A:77:GLU:HG2	1.48	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:HE2	1:B:75:LYS:HA	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:244:ASN:H	1:B:244:ASN:ND2	1.79	0.80
1:B:51:LYS:HD3	1:B:51:LYS:H	1.48	0.79
1:B:244:ASN:N	1:B:244:ASN:HD22	1.79	0.78
1:B:249:MET:HE3	1:B:261:ILE:HD13	1.66	0.78
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:B:249:MET:CE	1:B:261:ILE:HD13	2.17	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:110:PRO:HB2	1:B:151:LYS:HE2	1.76	0.67
1:B:272:ASP:HB2	1:B:275:LYS:HB2	1.77	0.67
1:A:11:ARG:HH21	1:A:12:ASN:HD21	1.41	0.67
1:B:281:TYR:CD1	1:B:281:TYR:N	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:B:100:THR:CG2	1:B:132:PRO:HB2	2.17	0.64
1:A:246:TYR:HB3	1:A:276:THR:HG21	1.79	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
1:B:277:LEU:HD23	1:B:278:THR:H	1.66	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:253:ARG:CB	1:A:281:TYR:HA	2.31	0.60
1:A:4:LYS:NZ	1:A:231:GLU:HG3	2.16	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:230:LEU:HD13	1:B:236:PHE:HA	1.85	0.59
1:B:126:LEU:HD12	1:B:131:ILE:HD12	1.83	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:280:GLY:O	1:A:281:TYR:CB	2.53	0.56
1:A:244:ASN:H	1:A:244:ASN:HD22	1.52	0.56
1:A:261:ILE:HG21	1:A:281:TYR:CD1	2.40	0.56
1:A:273:LEU:C	1:A:277:LEU:HD13	2.24	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:ND2	1:B:196:ASN:H	2.04	0.56
1:A:249:MET:CG	1:A:281:TYR:HB2	2.35	0.55
1:A:36:GLU:C	1:A:38:GLU:H	2.11	0.54
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:A:216:ILE:HG23	1:A:217:MET:N	2.23	0.53
1:B:24:PRO:HG2	1:B:83:PHE:HE1	1.74	0.53
1:B:143:GLY:O	1:B:147:LYS:HG3	2.09	0.53
1:A:199:SER:O	1:A:203:GLN:HB2	2.09	0.53
1:A:274:HIS:C	1:A:276:THR:H	2.11	0.53
1:A:210:ASN:N	1:A:210:ASN:ND2	2.53	0.53
1:A:253:ARG:NH1	1:A:281:TYR:CE1	2.77	0.52
1:A:2:GLY:HA2	1:A:235:GLU:OE2	2.09	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:B:253:ARG:HH21	1:B:261:ILE:HD12	1.75	0.51
1:A:194:THR:H	1:A:203:GLN:NE2	2.08	0.51
1:A:84:ASN:ND2	1:A:121:ASN:HD22	2.09	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:HD22	1:B:196:ASN:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG11	1:A:88:PHE:HZ	1.76	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: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:A:250:ASN:ND2	1:A:280:GLY:CA	2.76	0.48
1:A:274:HIS:HD2	1:A:316:ILE:HG23	1.78	0.48
1:A:62:ILE:O	1:A:65:LYS:HB2	2.14	0.48
1:B:249:MET:HB3	1:B:281:TYR:OH	2.13	0.48
1:B:207:SER:CB	1:B:211:LYS:O	2.62	0.48
1:B:249:MET:HE1	1:B:261:ILE:HD13	1.95	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: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:266:ILE:HD11	1:A:277:LEU:HD21	1.96	0.47
1:B:249:MET:HE3	1:B:261:ILE:HG21	1.97	0.47
1:A:166:ILE:HD11	1:A:173:LEU:HD21	1.97	0.47
1:A:7:LEU:HB3	1:A:286:GLU:HG3	1.96	0.47
1:B:70:ILE:HG23	1:B:71:ILE:H	1.79	0.47
1:B:275:LYS:C	1:B:277:LEU:H	2.19	0.46
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:316:ILE:C	1:A:318:LYS:H	2.19	0.46
1:B:73:GLU:O	1:B:75:LYS:N	2.49	0.46
1:A:149:TYR:CZ	1:B:106:ALA:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:166:ILE:CG2	1:A:166:ILE:O	2.64	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:B:129:LEU:O	1:B:130:ASN:C	2.55	0.45
1:B:174:LYS:HG3	1:B:224:MET:HE2	1.99	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:60:LYS:HE3	1:A:60:LYS:HB3	1.64	0.45
1:A:216:ILE:HG21	1:B:206:LEU:HD11	1.98	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:61:ASP:O	1:A:65:LYS:HD2	2.17	0.44
1:A:59:LYS:HB3	1:A:62:ILE:HG13	2.00	0.44
1:A:50:GLU:O	1:A:53:ILE:HG22	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: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:84:ASN:HD21	1:A:121:ASN:HD22	1.65	0.44
1:B:273:LEU:C	1:B:277:LEU:HD21	2.37	0.44
1:A:196:ASN:O	1:A:199:SER:HB3	2.17	0.43
1:A:192:VAL:HB	1:A:240:VAL:O	2.18	0.43
1:B:3:PHE:HE1	1:B:132:PRO:HB3	1.84	0.43
1:A:249:MET:SD	1:A:281:TYR:CD2	3.11	0.43
1:B:44:ILE:HG21	1:B:67:PRO:HG3	1.99	0.43
1:A:109:ILE:N	1:A:110:PRO:CD	2.81	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:10:ARG:HD3	1:A:132:PRO:HD2	2.00	0.43
1:B:54:ASN:HD21	1:B:60:LYS:HZ3	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLY:H	2:B:600:HMZ:HAH	1.84	0.42
1:A:200:ALA:O	1:A:201:ILE:C	2.58	0.42
1:B:225:SER:HB3	1:B:237:ILE:HD12	2.02	0.41
1:A:256:PHE:C	1:A:257:PRO:O	2.56	0.41
1:B:249:MET:SD	1:B:281:TYR:CZ	3.12	0.41
1:A:196:ASN:ND2	1:A:196:ASN:H	2.18	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:143:GLY:O	1:B:144:ASN:C	2.57	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:B:54:ASN:ND2	1:B:60:LYS:HZ1	2.18	0.41
1:B:54:ASN:HD21	1:B:60:LYS:NZ	2.18	0.41
1:A:275:LYS:HA	1:A:275:LYS:HD2	1.78	0.41
1:A:33:MET:HB2	1:A:82:PHE:CG	2.55	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 [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	316/323 (98%)	282 (89%)	25 (8%)	9 (3%)	6	2
1	B	316/323 (98%)	286 (90%)	25 (8%)	5 (2%)	12	6
All	All	632/646 (98%)	568 (90%)	50 (8%)	14 (2%)	8	3

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%)	258 (89%)	32 (11%)	8	4
1	B	290/295 (98%)	257 (89%)	33 (11%)	7	4
All	All	580/590 (98%)	515 (89%)	65 (11%)	7	4

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	34	LYS
1	A	56	VAL
1	A	62	ILE
1	A	65	LYS
1	A	71	ILE
1	A	72	ARG
1	A	75	LYS
1	A	83	PHE
1	A	95	ASN

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Mol	Chain	Res	Type
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	210	ASN
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	281	TYR
1	A	283	LYS
1	A	284	SER
1	A	304	LYS
1	A	318	LYS
1	B	10	ARG
1	B	14	ILE
1	B	27	LYS
1	B	30	GLU
1	B	46	LYS
1	B	48	LEU
1	B	51	LYS
1	B	55	ASN
1	B	57	SER
1	B	65	LYS
1	B	69	ASN
1	B	77	GLU
1	B	83	PHE
1	B	126	LEU
1	B	146	VAL
1	B	157	LEU
1	B	182	LYS
1	B	185	TYR
1	B	193	LYS
1	B	196	ASN

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Mol	Chain	Res	Type
1	B	206	LEU
1	B	210	ASN
1	B	230	LEU
1	B	244	ASN
1	B	249	MET
1	B	269	GLN
1	B	272	ASP
1	B	276	THR
1	B	279	ASN
1	B	288	ILE
1	B	308	MET
1	B	317	LEU
1	B	318	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	39	ASN
1	A	55	ASN
1	A	84	ASN
1	A	140	ASN
1	A	148	ASN
1	A	196	ASN
1	A	203	GLN
1	A	210	ASN
1	A	244	ASN
1	A	250	ASN
1	A	274	HIS
1	A	291	ASN
1	A	303	GLN
1	A	312	GLN
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	95	ASN
1	B	140	ASN
1	B	196	ASN
1	B	203	GLN

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Mol	Chain	Res	Type
1	B	219	GLN
1	B	244	ASN
1	B	269	GLN
1	B	279	ASN
1	B	291	ASN
1	B	312	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 carbohydrates 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	A	500	-	13,16,16	1.69	3 (23%)	18,21,21	1.98	3 (16%)
2	HMZ	B	600	-	13,16,16	1.75	3 (23%)	18,21,21	1.29	2 (11%)

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	A	500	-	-	0/9/11/11	0/1/1/1
2	HMZ	B	600	-	-	0/9/11/11	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HMZ	CAP-CAO	-2.46	1.37	1.41
2	A	500	HMZ	CAJ-CAM	2.31	1.54	1.51
2	A	500	HMZ	OAK-CAN	3.06	1.44	1.37
2	B	600	HMZ	CAP-CAM	3.50	1.55	1.48
2	B	600	HMZ	CAJ-CAM	3.86	1.57	1.51
2	A	500	HMZ	CAP-CAM	3.96	1.56	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HMZ	CAH-CAO-CAP	-2.70	118.28	120.63
2	B	600	HMZ	CAO-CAH-CAN	2.44	122.07	119.51
2	B	600	HMZ	CAO-CAP-CAM	3.55	123.18	120.25
2	A	500	HMZ	CAO-CAH-CAN	3.91	123.61	119.51
2	A	500	HMZ	CAO-CAP-CAM	6.22	125.40	120.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/323 (98%)	0.26	16 (5%) 32 41	30, 56, 88, 118	0
1	B	318/323 (98%)	0.58	36 (11%) 7 9	33, 63, 98, 111	0
All	All	636/646 (98%)	0.42	52 (8%) 14 20	30, 59, 94, 118	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	ILE	9.8
1	A	70	ILE	9.7
1	A	281	TYR	6.9
1	B	5	VAL	6.9
1	B	276	THR	5.5
1	B	280	GLY	5.3
1	B	317	LEU	5.2
1	B	70	ILE	5.0
1	A	72	ARG	5.0
1	A	271	GLY	5.0
1	B	13	ALA	4.7
1	B	277	LEU	4.7
1	B	274	HIS	4.3
1	A	73	GLU	4.2
1	B	71	ILE	4.1
1	B	255	TYR	4.0
1	A	272	ASP	3.9
1	B	316	ILE	3.7
1	A	255	TYR	3.7
1	A	258	ASN	3.7
1	B	315	ALA	3.6
1	B	72	ARG	3.6
1	A	67	PRO	3.4
1	B	314	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	251	TYR	3.2
1	B	281	TYR	3.1
1	B	284	SER	3.1
1	B	279	ASN	3.1
1	B	318	LYS	2.8
1	A	69	ASN	2.8
1	B	230	LEU	2.7
1	A	41	TYR	2.7
1	B	96	LYS	2.7
1	B	246	TYR	2.6
1	B	285	TYR	2.6
1	A	68	ASP	2.6
1	B	257	PRO	2.6
1	B	282	HIS	2.5
1	B	146	VAL	2.5
1	B	301	TYR	2.5
1	B	304	LYS	2.5
1	B	52	TYR	2.3
1	A	106	ALA	2.3
1	A	315	ALA	2.3
1	B	14	ILE	2.3
1	B	288	ILE	2.2
1	B	109	ILE	2.1
1	B	270	ASN	2.1
1	B	283	LYS	2.1
1	B	97	TYR	2.1
1	A	275	LYS	2.0
1	B	256	PHE	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	HMZ	A	500	16/16	0.65	0.30	4.90	60,77,84,85	0
2	HMZ	B	600	16/16	0.76	0.30	3.92	64,75,84,86	0
3	NA	B	325	1/1	0.90	0.08	-	95,95,95,95	0
3	NA	B	324	1/1	0.76	0.10	-	85,85,85,85	0
3	NA	A	324	1/1	0.84	0.26	-	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.