Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 AM GMT

PDB ID	:	3D4Z
Title	:	GOLGI MANNOSIDASE II complex with gluco-imidazole
Authors	:	Kuntz, D.A.; Tarling, C.A.; Withers, S.G.; Rose, D.R.
Deposited on	:	2008-05-15
Resolution	:	1.39 Å(reported)

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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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.
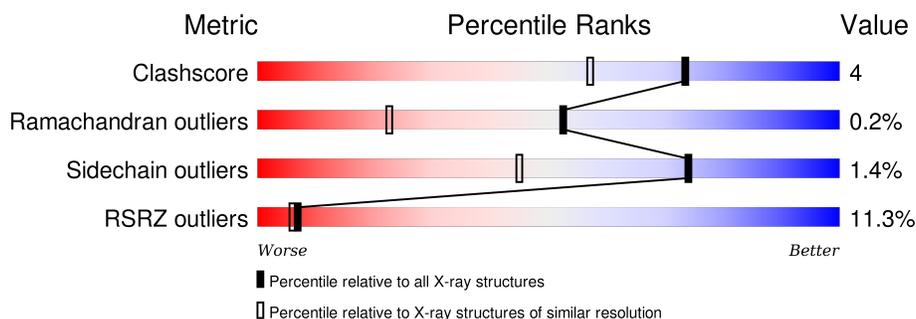
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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 <=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	1045	11% 86% 10% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9422 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 Alpha-mannosidase 2.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1016	8264	5256	1445	1522	41	0	9	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP Q24451
A	2	SER	-	EXPRESSION TAG	UNP Q24451
A	3	SER	-	EXPRESSION TAG	UNP Q24451
A	4	HIS	-	EXPRESSION TAG	UNP Q24451
A	5	HIS	-	EXPRESSION TAG	UNP Q24451
A	6	HIS	-	EXPRESSION TAG	UNP Q24451
A	7	HIS	-	EXPRESSION TAG	UNP Q24451
A	8	HIS	-	EXPRESSION TAG	UNP Q24451
A	9	HIS	-	EXPRESSION TAG	UNP Q24451
A	10	GLY	-	EXPRESSION TAG	UNP Q24451
A	11	GLU	-	EXPRESSION TAG	UNP Q24451
A	12	PHE	-	EXPRESSION TAG	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).
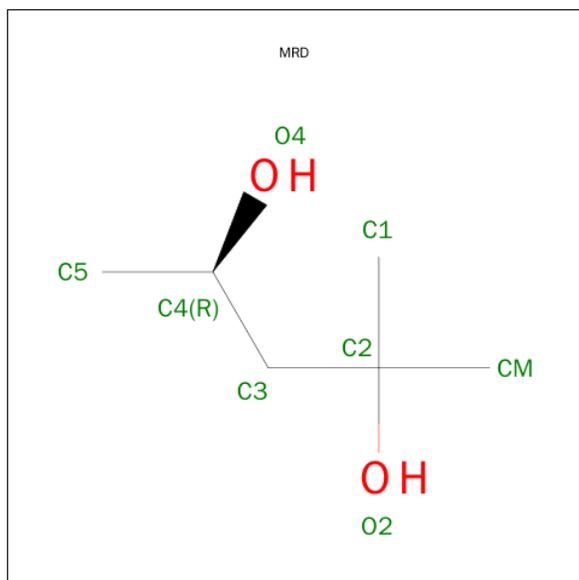
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0

- Molecule 4 is GLUCOIMIDAZOLE (three-letter code: GIM) (formula: $C_8H_{13}N_2O_4$).
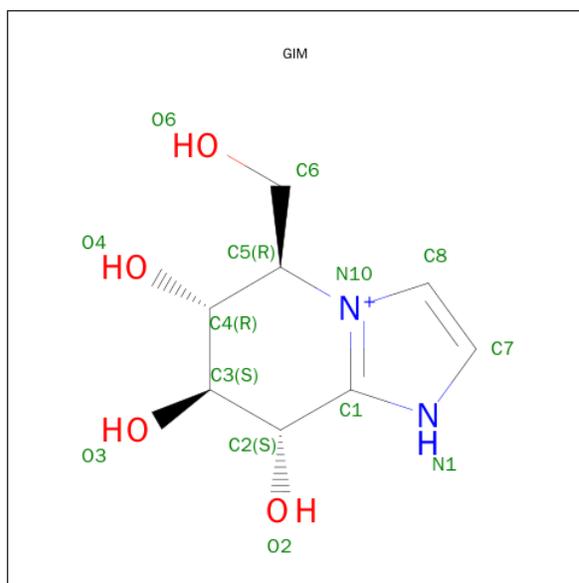
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 2	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1135	Total 1135	O 1135	0	6

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: Alpha-mannosidase 2
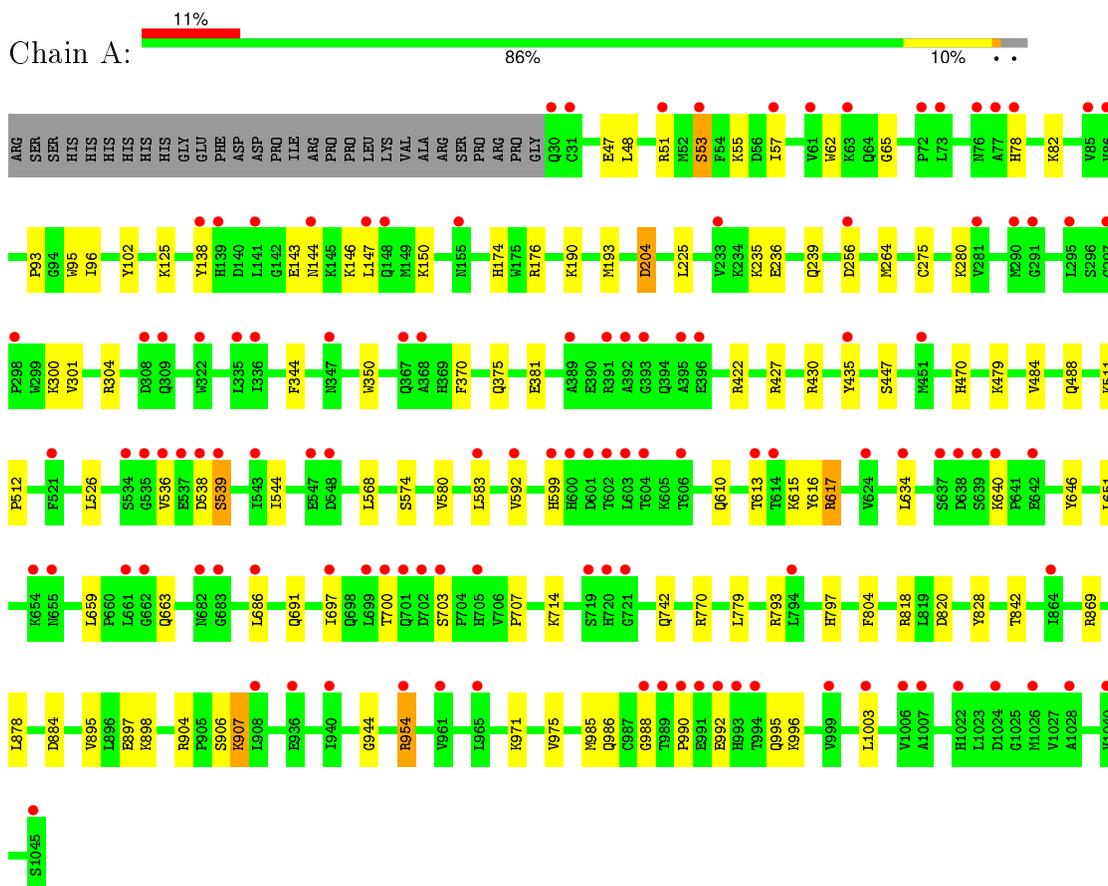
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.65Å 109.30Å 137.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.39 29.63 – 1.39	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-1.39) 94.7 (29.63-1.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 1.39Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.144 , 0.181 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 203042 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9422	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MRD, ZN, GIM

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	0.57	0/8500	1.09	15/11541 (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	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	793	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	422	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	617	ARG	CA-CB-CG	5.94	126.47	113.40
1	A	617	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	616	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	A	869	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	427	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	820	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	804	PHE	CB-CG-CD1	5.37	124.56	120.80
1	A	102	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	818	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	884	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	430	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	370	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	A	381	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	954	ARG	Sidechain

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	8264	0	8050	65	0
2	A	1	0	0	0	0
3	A	8	0	14	2	0
4	A	14	0	12	1	0
5	A	1135	0	0	20	0
All	All	9422	0	8076	67	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 4.

All (67) 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:A:583:LEU:O	1:A:583:LEU:HD23	1.77	0.84
1:A:907:LYS:H	1:A:907:LYS:HE2	1.49	0.77
1:A:651:LEU:HD22	1:A:659:LEU:HD11	1.68	0.76
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.71	0.70
1:A:256:ASP:HB2	5:A:1195:HOH:O	1.93	0.68
1:A:907:LYS:H	1:A:907:LYS:CE	2.06	0.68
1:A:742:GLN:HG3	5:A:1236:HOH:O	1.95	0.66
1:A:995:GLN:HG3	5:A:1372:HOH:O	1.96	0.65
3:A:1047:MRD:HMC3	5:A:1655:HOH:O	1.97	0.62
3:A:1047:MRD:HMC1	5:A:1654:HOH:O	1.99	0.62
1:A:280:LYS:HE3	1:A:301:VAL:HG21	1.83	0.60
1:A:954:ARG:NH1	5:A:1364:HOH:O	2.33	0.59
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.33	0.59
1:A:280:LYS:HE3	1:A:301:VAL:CG2	2.34	0.57
1:A:204:ASP:OD2	4:A:1048:GIM:H2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:LYS:HE3	5:A:1360:HOH:O	2.03	0.57
1:A:615:LYS:HD3	5:A:1446:HOH:O	2.04	0.56
1:A:904:ARG:HG2	1:A:985:MET:SD	2.46	0.56
1:A:714:LYS:HD2	5:A:1959:HOH:O	2.07	0.55
1:A:51:ARG:NH2	5:A:1067:HOH:O	2.40	0.54
1:A:907:LYS:N	1:A:907:LYS:HE2	2.20	0.53
1:A:53:SER:OG	1:A:55:LYS:HG2	2.09	0.52
1:A:988:GLY:O	1:A:990:PRO:HD3	2.10	0.52
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.45	0.51
1:A:47:GLU:HG2	5:A:1787:HOH:O	2.11	0.50
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.94	0.50
1:A:190:LYS:HE3	5:A:2057:HOH:O	2.12	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.49	0.48
1:A:544:ILE:HD13	1:A:574:SER:HB3	1.95	0.48
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.49	0.48
1:A:599:HIS:HB3	5:A:2161:HOH:O	2.14	0.47
1:A:640:LYS:HG2	1:A:646:TYR:CE1	2.50	0.47
1:A:700:THR:H	1:A:703:SER:HG	1.60	0.46
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.55	0.46
1:A:707:PRO:HG2	1:A:797:HIS:CE1	2.51	0.46
1:A:138[B]:TYR:CE2	1:A:146:LYS:HE2	2.50	0.46
1:A:986:GLN:NE2	5:A:1130:HOH:O	2.47	0.46
1:A:610:GLN:NE2	5:A:1449:HOH:O	2.49	0.46
1:A:96[A]:ILE:HD11	1:A:878:LEU:HA	1.97	0.46
1:A:82:LYS:HE2	5:A:1979:HOH:O	2.15	0.45
1:A:992:GLU:OE1	1:A:992:GLU:N	2.40	0.45
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.99	0.45
1:A:300:LYS:NZ	5:A:2014:HOH:O	2.50	0.44
1:A:615:LYS:NZ	5:A:1446:HOH:O	2.50	0.44
1:A:143:GLU:O	1:A:147:LEU:HG	2.18	0.44
1:A:583:LEU:HD22	1:A:944:GLY:HA3	1.99	0.43
1:A:235:LYS:O	1:A:239:GLN:HG3	2.18	0.43
1:A:842:THR:OG1	1:A:898:LYS:NZ	2.50	0.43
1:A:583:LEU:CD2	1:A:583:LEU:O	2.58	0.43
1:A:592:VAL:HA	1:A:617:ARG:O	2.19	0.43
1:A:613:THR:HG21	5:A:2103:HOH:O	2.19	0.43
1:A:150:LYS:HG2	1:A:193[A]:MET:CE	2.49	0.42
1:A:125:LYS:HE3	5:A:1094:HOH:O	2.18	0.42
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.01	0.42
1:A:907:LYS:NZ	1:A:907:LYS:H	2.16	0.42
1:A:971:LYS:HE2	1:A:971:LYS:HB2	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96[A]:ILE:HD12	1:A:479:LYS:HE2	2.02	0.41
1:A:538:ASP:OD1	1:A:538:ASP:O	2.37	0.41
1:A:536:VAL:HG22	1:A:779:LEU:HD11	2.02	0.41
1:A:511:LYS:HA	1:A:512:PRO:HD3	1.91	0.41
1:A:580:VAL:HG22	1:A:634:LEU:HD22	2.02	0.41
1:A:435[A]:TYR:CE2	1:A:526:LEU:HD13	2.56	0.41
1:A:304:ARG:HH11	1:A:304:ARG:HD2	1.70	0.41
1:A:344:PHE:HB3	1:A:350:TRP:CZ2	2.56	0.40
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.56	0.40
1:A:484:VAL:O	1:A:488:GLN:HG3	2.21	0.40
1:A:539:SER:OG	1:A:539:SER:O	2.30	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	1023/1045 (98%)	1000 (98%)	21 (2%)	2 (0%)	52	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	204	ASP

5.3.2 Protein sidechains (i)

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	911/929 (98%)	898 (99%)	13 (1%)	74 45

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	57	ILE
1	A	78	HIS
1	A	144	ASN
1	A	275	CYS
1	A	375	GLN
1	A	447	SER
1	A	539	SER
1	A	663	GLN
1	A	691	GLN
1	A	828	TYR
1	A	906	SER
1	A	907	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	643	HIS
1	A	993	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	#$|Z| > 2$
3	MRD	A	1047	-	6,7,7	0.25	0	7,10,10	0.62	0
4	GIM	A	1048	2	11,15,15	0.81	0	12,22,22	2.31	7 (58%)

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
3	MRD	A	1047	-	-	0/5/5/5	0/0/0/0
4	GIM	A	1048	2	-	0/2/22/22	0/1/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1048	GIM	C8-N10-C1	-3.84	105.42	109.05
4	A	1048	GIM	C6-C5-C4	-3.25	106.35	112.50
4	A	1048	GIM	C1-C2-C3	-2.86	107.50	113.17
4	A	1048	GIM	C4-C3-C2	-2.49	107.95	110.72
4	A	1048	GIM	O4-C4-C5	-2.04	106.15	109.82
4	A	1048	GIM	C3-C4-C5	2.02	114.11	111.39
4	A	1048	GIM	O2-C2-C1	3.34	114.80	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1047	MRD	2	0
4	A	1048	GIM	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1016/1045 (97%)	0.95	115 (11%)	7	6	7, 14, 31, 69	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	10.9
1	A	536	VAL	10.3
1	A	993	HIS	9.7
1	A	539	SER	8.5
1	A	602	THR	7.6
1	A	537	GLU	7.4
1	A	702	ASP	7.3
1	A	78	HIS	7.1
1	A	720	HIS	7.1
1	A	638	ASP	7.0
1	A	534	SER	6.8
1	A	989	THR	6.3
1	A	703	SER	6.2
1	A	682	ASN	5.6
1	A	701	GLN	5.5
1	A	639	SER	5.3
1	A	521	PHE	5.1
1	A	655	ASN	5.1
1	A	538	ASP	4.8
1	A	297	CYS	4.8
1	A	600	HIS	4.7
1	A	77	ALA	4.6
1	A	147	LEU	4.4
1	A	535	GLY	4.3
1	A	583	LEU	4.2
1	A	700	THR	4.2
1	A	31	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	990	PRO	4.1
1	A	57	ILE	3.9
1	A	139	HIS	3.9
1	A	683	GLY	3.8
1	A	606	THR	3.7
1	A	601	ASP	3.7
1	A	614	THR	3.7
1	A	290	MET	3.6
1	A	392	ALA	3.6
1	A	30	GLN	3.4
1	A	662	GLY	3.4
1	A	992	GLU	3.3
1	A	908	LEU	3.2
1	A	994	THR	3.2
1	A	395	ALA	3.1
1	A	72	PRO	3.1
1	A	322	TRP	3.0
1	A	73	LEU	3.0
1	A	1024	ASP	3.0
1	A	368	ALA	3.0
1	A	335	LEU	3.0
1	A	1022	HIS	2.9
1	A	76	ASN	2.9
1	A	697	ILE	2.9
1	A	991	GLU	2.9
1	A	547	GLU	2.8
1	A	592	VAL	2.8
1	A	599	HIS	2.7
1	A	721	GLY	2.7
1	A	999	VAL	2.7
1	A	1026	MET	2.7
1	A	451	MET	2.7
1	A	954	ARG	2.6
1	A	309	GLN	2.6
1	A	138[A]	TYR	2.6
1	A	1040	VAL	2.6
1	A	988	GLY	2.6
1	A	347	ASN	2.5
1	A	543	ILE	2.5
1	A	940	ILE	2.5
1	A	144	ASN	2.5
1	A	391	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	295	LEU	2.5
1	A	336	ILE	2.5
1	A	256	ASP	2.5
1	A	1045	SER	2.5
1	A	393	GLY	2.4
1	A	141	LEU	2.4
1	A	686	LEU	2.4
1	A	604	THR	2.4
1	A	661	LEU	2.4
1	A	961	VAL	2.4
1	A	51	ARG	2.3
1	A	637	SER	2.3
1	A	281	VAL	2.3
1	A	435[A]	TYR	2.3
1	A	389	ALA	2.3
1	A	1028	ALA	2.3
1	A	864	ILE	2.3
1	A	396	GLU	2.3
1	A	308	ASP	2.3
1	A	699	LEU	2.3
1	A	634	LEU	2.3
1	A	1007	ALA	2.2
1	A	233	VAL	2.2
1	A	298	PRO	2.2
1	A	719	SER	2.2
1	A	936	GLU	2.2
1	A	624	VAL	2.2
1	A	291	GLY	2.2
1	A	1003	LEU	2.2
1	A	148	GLN	2.2
1	A	705	HIS	2.1
1	A	654	LYS	2.1
1	A	367	GLN	2.1
1	A	61	VAL	2.1
1	A	640	LYS	2.1
1	A	85	VAL	2.1
1	A	86	VAL	2.1
1	A	1006	VAL	2.1
1	A	548	ASP	2.1
1	A	642	GLU	2.1
1	A	53	SER	2.1
1	A	63	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	965	LEU	2.1
1	A	613	THR	2.0
1	A	155	ASN	2.0
1	A	794	LEU	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
4	GIM	A	1048	14/14	0.95	0.10	1.47	7,9,10,10	0
3	MRD	A	1047	8/8	0.72	0.18	1.46	14,18,27,27	0
2	ZN	A	1046	1/1	1.00	0.07	-1.83	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.