



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:57 PM UTC

PDB ID : 3BUI / pdb_00003bui
Title : Golgi mannosidase II D204A catalytic nucleophile mutant complex with Tris
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2008-01-02
Resolution : 1.25 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

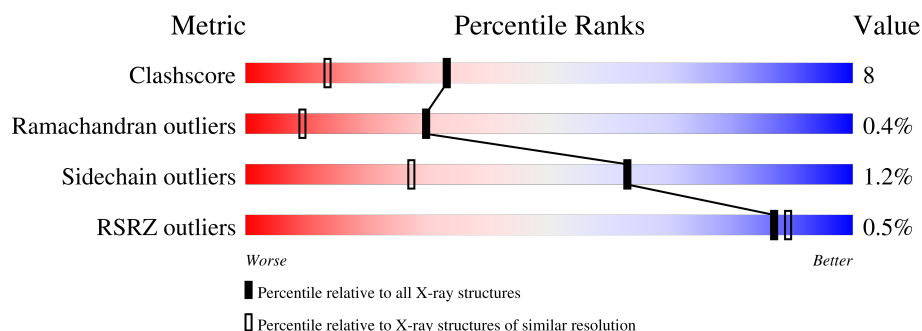
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	1045	

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
4	MPD	A	1048	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10090 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
1	A	1016	Total	C	N	O	S	0	50	0
			8543	5444	1495	1559	45			

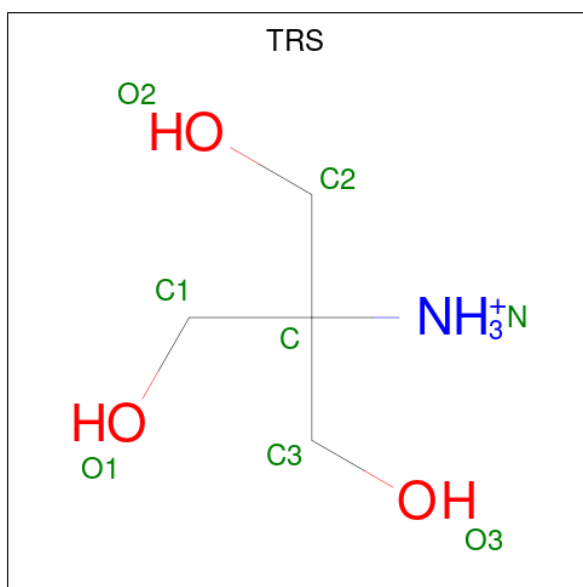
There are 14 discrepancies between the modelled and reference sequences:

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	204	ALA	ASP	engineered mutation	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

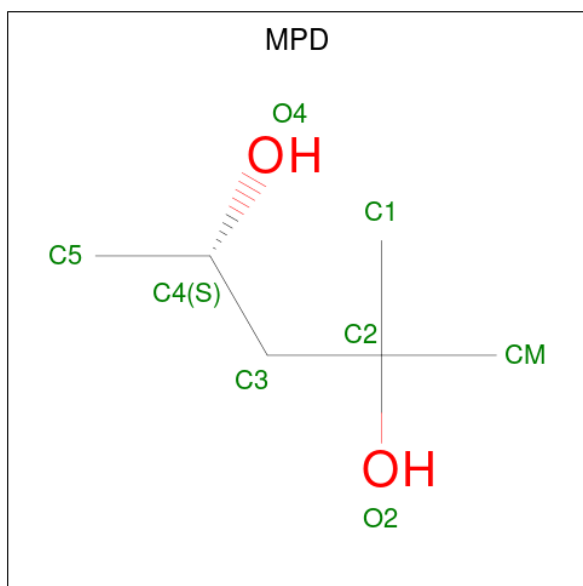
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			9	4	1	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

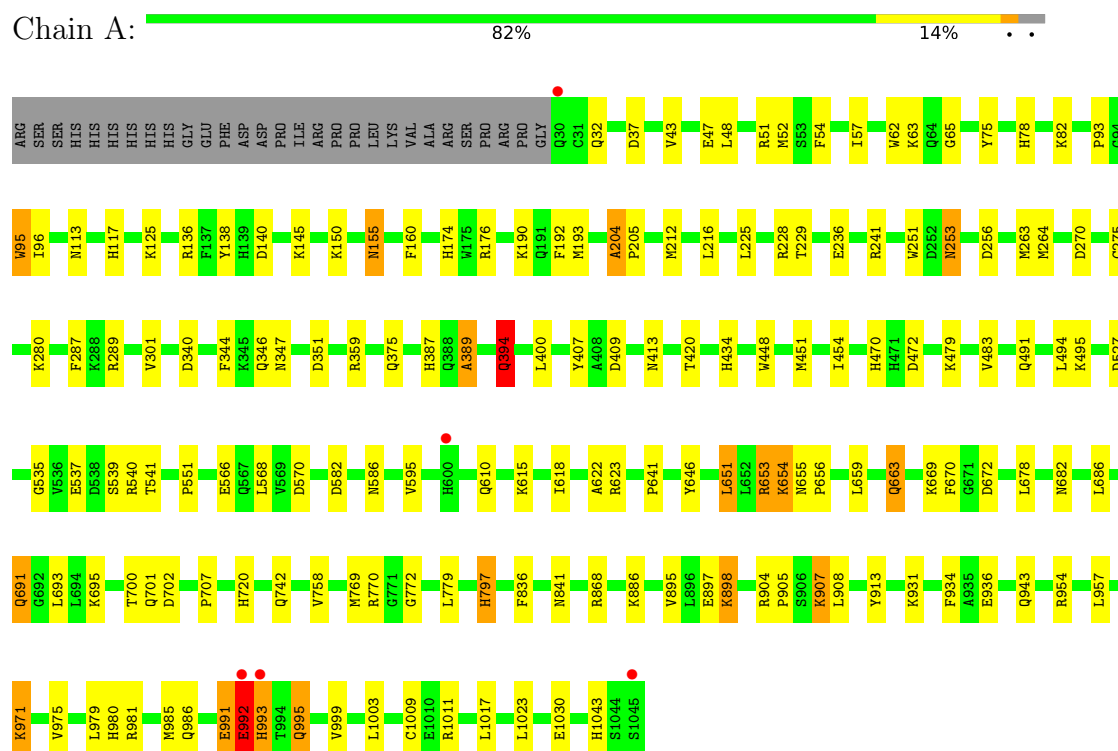
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1502	Total	O	0	43
			1505	1505		

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: Alpha-mannosidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.26Å 108.99Å 137.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.25 10.00 – 1.25	Depositor EDS
% Data completeness (in resolution range)	91.8 (10.00-1.25) 89.6 (10.00-1.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 1.25Å)	Xtriage
Refinement program	SHELXL-97, CNS, SHELX	Depositor
R, R_{free}	0.121 , 0.159 0.115 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10090	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MPD, TRS

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	0.80	1/8863 (0.0%)	1.31	53/12022 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	772	GLY	N-CA	5.71	1.50	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ASN	OD1-CG-ND2	-11.80	110.80	122.60
1	A	995	GLN	OE1-CD-NE2	10.47	133.07	122.60
1	A	394	GLN	OE1-CD-NE2	9.85	132.45	122.60
1	A	347	ASN	OD1-CG-ND2	9.31	131.91	122.60
1	A	155	ASN	CB-CG-ND2	8.08	128.52	116.40
1	A	986	GLN	CA-C-O	-7.77	111.82	120.60
1	A	253	ASN	OD1-CG-ND2	7.22	129.82	122.60
1	A	347	ASN	CA-CB-CG	-6.99	105.61	112.60
1	A	670	PHE	CA-CB-CG	-6.93	106.87	113.80
1	A	682	ASN	O-C-N	6.83	130.66	122.26
1	A	78	HIS	CA-CB-CG	-6.64	107.16	113.80
1	A	992	GLU	CA-C-N	6.51	133.97	121.54
1	A	992	GLU	C-N-CA	6.51	133.97	121.54
1	A	836	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	434	HIS	CA-CB-CG	-6.35	107.45	113.80
1	A	992	GLU	CB-CA-C	-6.29	107.36	116.54
1	A	980	HIS	CA-CB-CG	-6.19	107.61	113.80
1	A	287	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	797[A]	HIS	CA-CB-CG	6.02	119.82	113.80
1	A	797[B]	HIS	CA-CB-CG	6.02	119.82	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	PRO	CB-CA-C	-5.90	103.22	110.95
1	A	663	GLN	CB-CG-CD	-5.84	102.68	112.60
1	A	995	GLN	CG-CD-NE2	-5.83	107.65	116.40
1	A	992	GLU	N-CA-C	5.77	116.82	108.34
1	A	155	ASN	CA-CB-CG	5.74	118.34	112.60
1	A	663	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	A	160	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	1030	GLU	CA-C-O	5.55	128.31	121.87
1	A	387	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	344	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	646	TYR	CA-CB-CG	-5.50	104.00	113.90
1	A	413	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	841	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	943	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	A	610	GLN	CA-C-N	-5.41	116.53	122.38
1	A	610	GLN	C-N-CA	-5.41	116.53	122.38
1	A	991	GLU	CA-C-N	-5.38	114.20	121.84
1	A	991	GLU	C-N-CA	-5.38	114.20	121.84
1	A	192	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	270	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	113	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	389	ALA	CA-C-O	5.29	126.16	120.55
1	A	586	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	682	ASN	N-CA-C	-5.22	106.22	112.59
1	A	389	ALA	O-C-N	-5.17	116.64	122.12
1	A	610	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	655	ASN	CA-CB-CG	-5.17	107.43	112.60
1	A	340	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	1043	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	623	ARG	CD-NE-CZ	-5.05	117.32	124.40
1	A	409	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	289	ARG	CA-C-N	-5.01	114.27	122.54
1	A	289	ARG	C-N-CA	-5.01	114.27	122.54

There are no chirality outliers.

There are no planarity outliers.

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	8543	0	8399	126	0
2	A	1	0	0	0	0
3	A	9	0	6	0	0
4	A	32	0	56	8	0
5	A	1505	0	0	58	0
All	All	10090	0	8461	133	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 8.

All (133) 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:96[A]:ILE:HG22	5:A:2357:HOH:O	1.50	1.10
1:A:96[A]:ILE:HG23	1:A:479:LYS:HE2	1.65	0.79
1:A:57:ILE:HD11	5:A:2218:HOH:O	1.84	0.78
1:A:241[B]:ARG:CZ	5:A:1586:HOH:O	2.30	0.77
1:A:136[B]:ARG:HD2	5:A:1202[B]:HOH:O	1.88	0.72
1:A:541:THR:HG23	5:A:2332:HOH:O	1.89	0.71
1:A:253:ASN:ND2	5:A:2010:HOH:O	2.23	0.70
1:A:491:GLN:HG3	1:A:495:LYS:HE2	1.74	0.69
1:A:125:LYS:HE3	5:A:1562:HOH:O	1.91	0.69
1:A:145:LYS:HE3	5:A:2049:HOH:O	1.92	0.69
1:A:693:LEU:HD13	5:A:1082:HOH:O	1.92	0.69
1:A:663:GLN:HG3	5:A:1393:HOH:O	1.96	0.66
1:A:720:HIS:CE1	5:A:2393:HOH:O	2.49	0.66
1:A:96[B]:ILE:HD12	5:A:2427:HOH:O	1.96	0.65
1:A:136[B]:ARG:NH2	1:A:140:ASP:OD2	2.30	0.65
1:A:82[B]:LYS:CE	5:A:1272:HOH:O	2.43	0.64
1:A:491:GLN:OE1	4:A:1049:MPD:HM3	1.98	0.64
4:A:1049:MPD:H53	5:A:2263[B]:HOH:O	1.97	0.64
1:A:551:PRO:HG2	5:A:2144:HOH:O	1.99	0.62
1:A:651:LEU:HD13	1:A:653:ARG:HG2	1.82	0.62
1:A:908:LEU:HB3	5:A:2543:HOH:O	2.00	0.61
1:A:82[A]:LYS:HD2	1:A:375[A]:GLN:HE22	1.66	0.60
1:A:653:ARG:HD3	1:A:654:LYS:O	2.02	0.60
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.37	0.59
1:A:138[A]:TYR:OH	1:A:150:LYS:HE2	2.02	0.59
1:A:934:PHE:CE2	1:A:936[A]:GLU:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LEU:HB3	5:A:2336:HOH:O	2.03	0.59
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.43	0.58
1:A:707:PRO:HG2	1:A:797[A]:HIS:CD2	2.38	0.58
1:A:47:GLU:OE2	1:A:51:ARG:HD3	2.03	0.58
1:A:256:ASP:HB2	5:A:2017:HOH:O	2.02	0.58
1:A:494:LEU:HB3	4:A:1049:MPD:HM1	1.84	0.58
1:A:653:ARG:HD2	1:A:656:PRO:HA	1.85	0.57
1:A:483:VAL:HG11	5:A:2463:HOH:O	2.04	0.57
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.33	0.57
1:A:979[A]:LEU:HD21	1:A:999:VAL:HG11	1.87	0.57
1:A:491:GLN:HG3	1:A:495:LYS:CE	2.35	0.57
1:A:96[A]:ILE:HG21	5:A:2427:HOH:O	2.05	0.57
1:A:527:ASP:O	1:A:931:LYS:HE3	2.06	0.55
1:A:975:VAL:HG21	1:A:1003:LEU:HD22	1.87	0.55
1:A:936[A]:GLU:HG3	5:A:2183:HOH:O	2.05	0.55
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.87	0.55
1:A:701:GLN:HG3	5:A:1350:HOH:O	2.07	0.54
1:A:971[A]:LYS:NZ	1:A:971[A]:LYS:HB2	2.21	0.54
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.89	0.54
1:A:975:VAL:HG21	1:A:1003:LEU:CD2	2.38	0.53
1:A:228[A]:ARG:HD3	1:A:407:TYR:CE2	2.43	0.53
4:A:1049:MPD:HM2	4:A:1049:MPD:H52	1.89	0.53
1:A:654:LYS:HE3	1:A:672:ASP:OD1	2.08	0.53
1:A:905:PRO:HD3	1:A:985[B]:MET:HE1	1.89	0.53
1:A:82[A]:LYS:NZ	5:A:1272:HOH:O	2.40	0.53
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.43	0.53
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	1.92	0.53
1:A:913:TYR:HB2	1:A:985[B]:MET:HE3	1.90	0.53
1:A:280:LYS:HE2	1:A:301:VAL:HG21	1.91	0.52
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.50	0.52
4:A:1049:MPD:H51	5:A:1488:HOH:O	2.10	0.52
1:A:540:ARG:HB2	5:A:2319:HOH:O	2.09	0.52
1:A:695:LYS:HD3	5:A:2326:HOH:O	2.10	0.52
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:HD2	1.74	0.52
1:A:95:TRP:CE3	1:A:96[A]:ILE:HG12	2.45	0.51
1:A:904:ARG:HA	1:A:985[B]:MET:HE1	1.92	0.51
1:A:451:MET:HE2	5:A:2433:HOH:O	2.10	0.51
1:A:1011:ARG:HD2	5:A:1300:HOH:O	2.11	0.51
1:A:678:LEU:HD12	1:A:769[B]:MET:HE1	1.93	0.51
1:A:686:LEU:HG	1:A:769[A]:MET:HE3	1.92	0.51
1:A:32:GLN:HG3	5:A:2527:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212[B]:MET:HG3	1:A:216:LEU:CD1	2.42	0.49
1:A:451:MET:CE	5:A:2433:HOH:O	2.60	0.49
1:A:957:LEU:HD11	1:A:979[B]:LEU:HG	1.92	0.49
1:A:678:LEU:CD1	1:A:769[B]:MET:HE1	2.43	0.49
1:A:212[B]:MET:HG2	5:A:1725:HOH:O	2.13	0.49
1:A:280:LYS:HE2	1:A:301:VAL:CG2	2.42	0.49
1:A:907:LYS:HB2	1:A:907:LYS:NZ	2.28	0.49
1:A:63:LYS:HE2	5:A:2261:HOH:O	2.13	0.48
1:A:742[A]:GLN:HG3	5:A:1087:HOH:O	2.13	0.48
1:A:700:THR:HA	5:A:2435:HOH:O	2.14	0.48
1:A:720:HIS:ND1	5:A:2393:HOH:O	2.34	0.48
1:A:82[B]:LYS:HE2	5:A:1272:HOH:O	2.07	0.48
4:A:1050:MPD:H13	5:A:1717:HOH:O	2.12	0.48
1:A:57:ILE:HG12	5:A:1135:HOH:O	2.13	0.48
4:A:1050:MPD:HM3	5:A:1191:HOH:O	2.14	0.47
4:A:1051:MPD:O4	4:A:1051:MPD:H11	2.14	0.47
1:A:51:ARG:HG3	5:A:1744:HOH:O	2.15	0.47
1:A:669:LYS:HD3	5:A:1370:HOH:O	2.14	0.47
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.49	0.47
1:A:155:ASN:HB3	5:A:1250:HOH:O	2.14	0.46
1:A:47:GLU:CD	1:A:51:ARG:HD3	2.41	0.46
1:A:52[A]:MET:HE2	1:A:54:PHE:CZ	2.50	0.46
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:CD	2.29	0.46
1:A:886:LYS:NZ	5:A:1483:HOH:O	2.48	0.46
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.96	0.46
1:A:346[A]:GLN:NE2	5:A:2388:HOH:O	2.49	0.46
1:A:136[B]:ARG:HH21	1:A:140:ASP:CG	2.24	0.46
1:A:37:ASP:HB2	5:A:2498:HOH:O	2.16	0.45
1:A:96[A]:ILE:CG2	5:A:2357:HOH:O	2.31	0.45
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:NE	2.14	0.45
1:A:570:ASP:HA	1:A:618:ILE:O	2.17	0.45
1:A:971[A]:LYS:NZ	5:A:1448:HOH:O	2.49	0.45
1:A:993:HIS:O	1:A:993:HIS:ND1	2.49	0.45
1:A:251:TRP:CD1	1:A:251:TRP:C	2.95	0.45
1:A:43:VAL:O	1:A:400:LEU:HA	2.17	0.44
1:A:470:HIS:CD2	1:A:472:ASP:H	2.35	0.44
1:A:359:ARG:NE	5:A:1634:HOH:O	2.50	0.44
1:A:228[B]:ARG:HG3	5:A:2551:HOH:O	2.16	0.43
1:A:229:THR:HG21	1:A:263:MET:HE2	2.01	0.43
1:A:535:GLY:HA3	1:A:779:LEU:HD21	2.00	0.43
1:A:582:ASP:HB2	5:A:2275:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ALA:O	1:A:394:GLN:HB2	2.19	0.43
1:A:898:LYS:HA	1:A:898:LYS:HD2	1.85	0.42
1:A:541:THR:HG21	5:A:2172:HOH:O	2.19	0.42
1:A:595:VAL:HG21	1:A:615:LYS:HG3	2.01	0.42
1:A:566:GLU:HA	1:A:622:ALA:O	2.19	0.42
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.60	0.42
1:A:992:GLU:OE2	1:A:992:GLU:HA	2.18	0.42
1:A:448:TRP:CG	1:A:454:ILE:HG13	2.55	0.42
1:A:228[A]:ARG:HB2	5:A:2551:HOH:O	2.19	0.41
1:A:537:GLU:HG2	1:A:539:SER:HB3	2.00	0.41
1:A:241[B]:ARG:NE	5:A:1586:HOH:O	2.47	0.41
1:A:995:GLN:N	5:A:1898:HOH:O	2.53	0.41
1:A:981[A]:ARG:NH2	5:A:1332:HOH:O	2.52	0.41
1:A:420:THR:HB	1:A:868:ARG:HD2	2.03	0.41
1:A:75[B]:TYR:HD2	5:A:1574:HOH:O	2.03	0.40
1:A:535:GLY:HA3	1:A:779:LEU:CD2	2.51	0.40
1:A:691:GLN:O	1:A:758:VAL:HG21	2.22	0.40
1:A:770:ARG:HH11	1:A:770:ARG:HD2	1.74	0.40
1:A:979[B]:LEU:HD22	5:A:2465:HOH:O	2.21	0.40
1:A:47:GLU:OE2	1:A:51:ARG:CD	2.68	0.40
1:A:150:LYS:HG2	1:A:193[A]:MET:CE	2.51	0.40
1:A:212[B]:MET:HG3	1:A:216:LEU:HD11	2.03	0.40
1:A:190:LYS:NZ	1:A:1017:LEU:O	2.49	0.40
1:A:204:ALA:H	1:A:205:PRO:HD3	1.86	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	1064/1045 (102%)	1037 (98%)	23 (2%)	4 (0%)	30 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	993	HIS
1	A	991	GLU
1	A	204	ALA

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	952/928 (103%)	940 (99%)	12 (1%)	61 24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	394	GLN
1	A	651	LEU
1	A	653	ARG
1	A	654	LYS
1	A	691	GLN
1	A	702	ASP
1	A	898	LYS
1	A	907	LYS
1	A	971[A]	LYS
1	A	971[B]	LYS
1	A	992	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	249	GLN
1	A	371	ASN
1	A	778	ASN

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Mol	Chain	Res	Type
1	A	812	GLN
1	A	866	GLN
1	A	1005	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
4	MPD	A	1048	-	7,7,7	0.62	0	9,10,10	0.93	0
3	TRS	A	1047[B]	-	7,7,7	1.29	1 (14%)	9,9,9	2.91	4 (44%)
3	TRS	A	1047[A]	-	7,7,7	1.09	0	9,9,9	1.94	4 (44%)
4	MPD	A	1051	-	7,7,7	0.59	0	9,10,10	0.53	0
4	MPD	A	1049	-	7,7,7	0.35	0	9,10,10	0.84	0
4	MPD	A	1050	-	7,7,7	0.35	0	9,10,10	0.76	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
4	MPD	A	1048	-	1/1/2/2	3/5/5/5	-
3	TRS	A	1047[B]	-	-	3/9/9/9	-
3	TRS	A	1047[A]	-	-	0/9/9/9	-
4	MPD	A	1051	-	-	1/5/5/5	-
4	MPD	A	1049	-	-	4/5/5/5	-
4	MPD	A	1050	-	-	4/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1047[B]	TRS	O1-C1	2.12	1.49	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1047[B]	TRS	O1-C1-C	-6.85	91.79	110.88
3	A	1047[A]	TRS	C1-C-N	-3.64	98.90	108.17
3	A	1047[B]	TRS	C1-C-N	-3.64	98.90	108.17
3	A	1047[A]	TRS	C2-C-C1	2.55	117.45	110.66
3	A	1047[B]	TRS	C2-C-C1	2.55	117.45	110.66
3	A	1047[A]	TRS	O3-C3-C	-2.44	104.08	110.88
3	A	1047[B]	TRS	O3-C3-C	-2.44	104.08	110.88
3	A	1047[A]	TRS	O1-C1-C	-2.17	104.84	110.88

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1048	MPD	C4

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1047[B]	TRS	C2-C-C1-O1
3	A	1047[B]	TRS	C3-C-C1-O1
3	A	1047[B]	TRS	N-C-C1-O1
4	A	1048	MPD	C2-C3-C4-O4
4	A	1048	MPD	C2-C3-C4-C5
4	A	1049	MPD	C1-C2-C3-C4
4	A	1049	MPD	C2-C3-C4-O4
4	A	1049	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	1050	MPD	C1-C2-C3-C4
4	A	1050	MPD	O2-C2-C3-C4
4	A	1050	MPD	CM-C2-C3-C4
4	A	1050	MPD	C2-C3-C4-C5
4	A	1048	MPD	O2-C2-C3-C4
4	A	1051	MPD	O2-C2-C3-C4
4	A	1049	MPD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1051	MPD	1	0
4	A	1049	MPD	5	0
4	A	1050	MPD	2	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%)	-0.68	5 (0%) 87 89	4, 11, 28, 67	50 (4%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	3.5
1	A	600	HIS	3.3
1	A	992	GLU	2.8
1	A	30	GLN	2.2
1	A	1045	SER	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(Å ²)	Q<0.9
4	MPD	A	1049	8/8	0.75	0.13	52,55,58,60	0
4	MPD	A	1050	8/8	0.78	0.12	44,51,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MPD	A	1051	8/8	0.82	0.11	23,28,43,43	0
3	TRS	A	1047[B]	8/8	0.95	0.06	12,15,16,17	1
3	TRS	A	1047[A]	8/8	0.95	0.06	11,15,16,17	1
4	MPD	A	1048	8/8	0.98	0.04	11,15,19,20	0
2	ZN	A	1046	1/1	1.00	0.01	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.