



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 4WVC / pdb_00004wvc
Title : Crystal structure of GH63 mannosylglycerate hydrolase from *Thermus thermophilus* HB8 in complex with Tris and D-glycerate
Authors : Miyazaki, T.; Ichikawa, M.; Nishikawa, A.; Tonozuka, T.
Deposited on : 2014-11-05
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

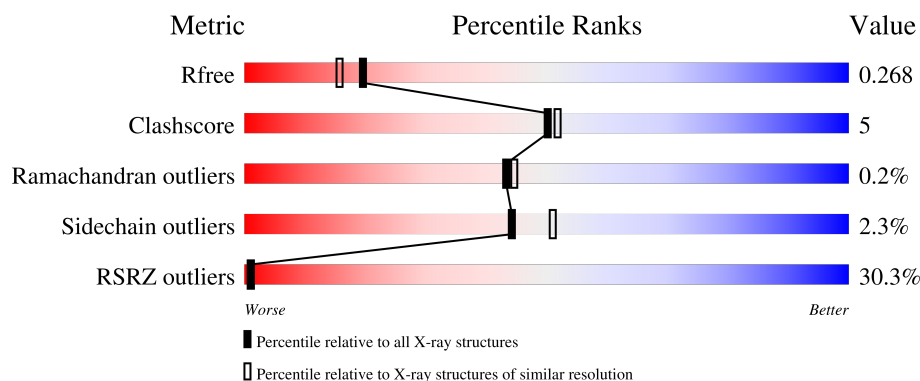
1 Overall quality at a glance

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	420	5% 88% 10% .
1	B	420	54% 82% 14% ..

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
3	TRS	A	501	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7093 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.

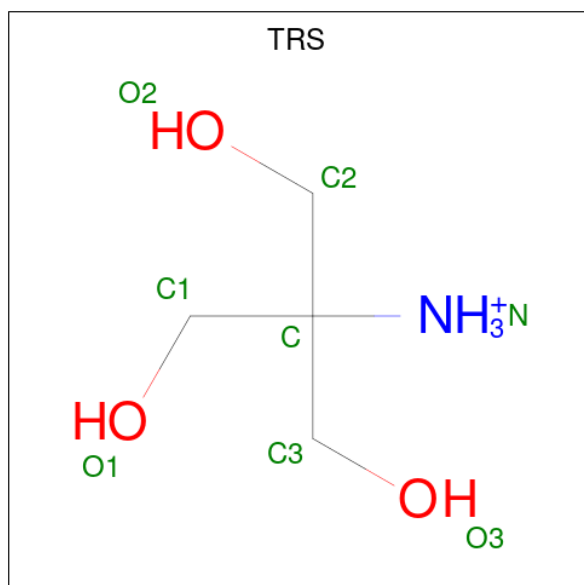
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3416	2215	598	598	5			
1	B	409	Total	C	N	O	S	0	0	0
			3380	2191	590	594	5			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

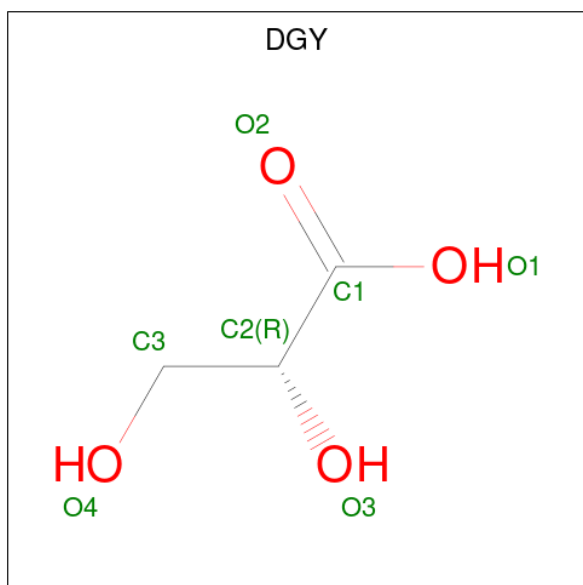
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- 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	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is (2R)-2,3-DIHYDROXYPROPANOIC ACID (CCD ID: DGY) (formula: $C_3H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

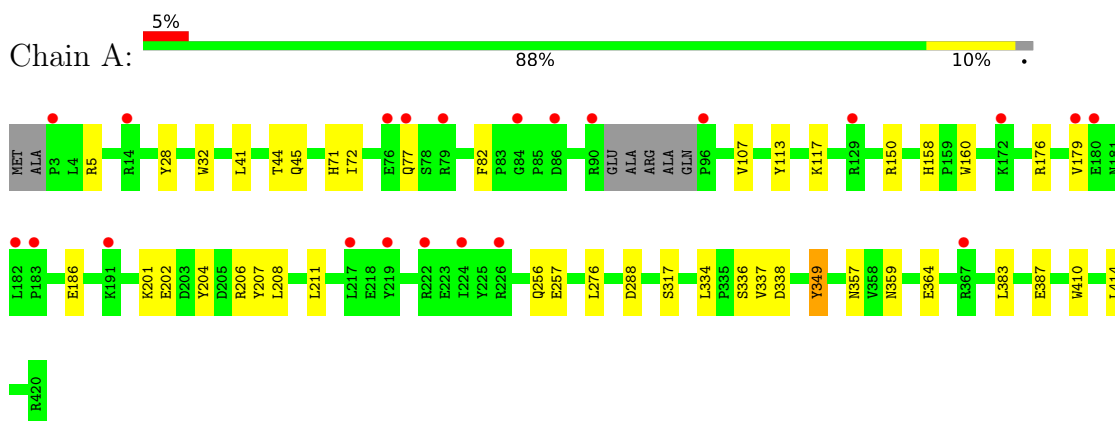
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total	O	0	0
			145	145		
5	B	120	Total	O	0	0
			120	120		

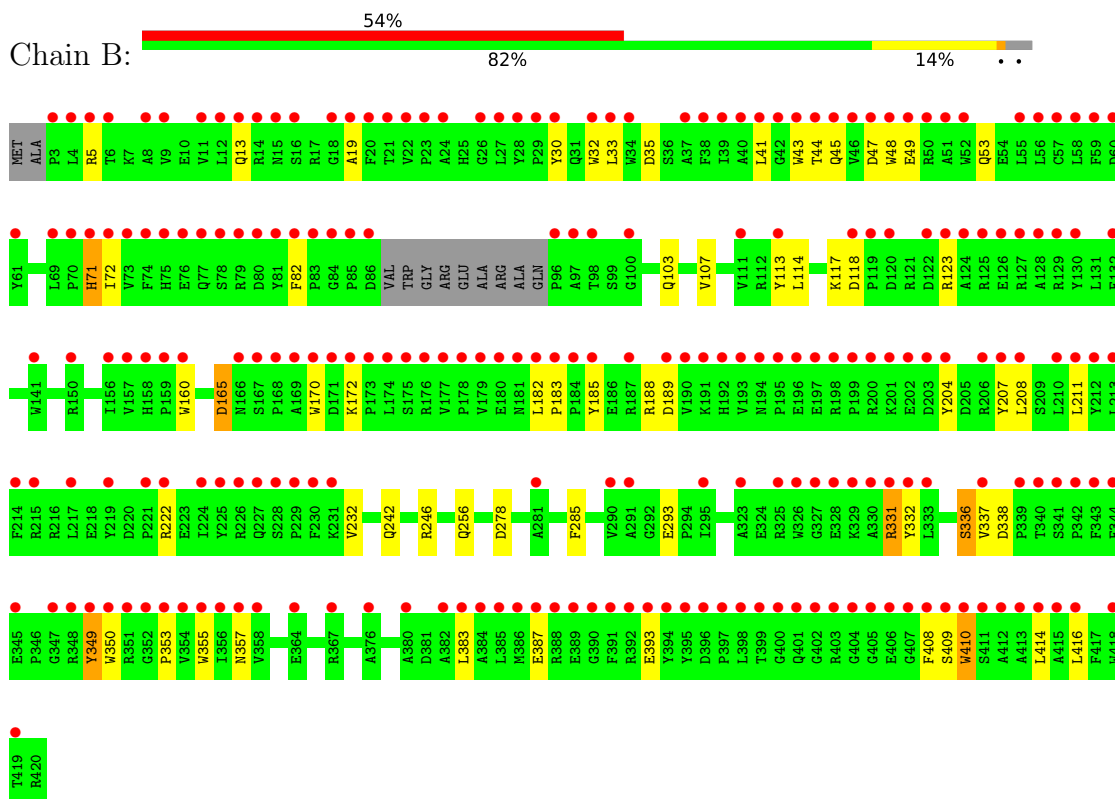
3 Residue-property plots [i](#)

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.94Å 92.94Å 190.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.15 – 2.10 45.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.15-2.10) 98.9 (45.15-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.245 , 0.280 0.256 , 0.268	Depositor DCC
R_{free} test set	3437 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7093	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: DGY, TRS, CL

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	0.70	0/3535	0.85	1/4818 (0.0%)
1	B	0.70	0/3497	0.89	5/4766 (0.1%)
All	All	0.70	0/7032	0.87	6/9584 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	PRO	CA-C-N	-6.05	113.30	119.83
1	B	183	PRO	C-N-CA	-6.05	113.30	119.83
1	B	409	SER	N-CA-C	5.95	117.43	111.07
1	B	107	VAL	N-CA-C	5.74	115.93	110.42
1	B	165	ASP	N-CA-C	5.73	117.52	111.28
1	A	107	VAL	N-CA-C	5.09	115.30	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3280	24	0
1	B	3380	0	3245	49	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	8	0	12	1	0
3	B	8	0	12	0	0
4	A	7	0	5	0	0
4	B	7	0	5	1	0
5	A	145	0	0	4	0
5	B	120	0	0	15	1
All	All	7093	0	6559	71	1

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 5.

All (71) 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:257:GLU:OE1	1:B:222:ARG:NE	1.97	0.95
1:A:201:LYS:HG3	5:A:711:HOH:O	1.89	0.73
1:A:364:GLU:HB3	5:A:635:HOH:O	1.90	0.72
1:B:47:ASP:HB3	5:B:652:HOH:O	1.89	0.71
1:B:165:ASP:HB3	5:B:705:HOH:O	1.92	0.68
1:B:43:TRP:HE3	5:B:652:HOH:O	1.77	0.68
1:B:19:ALA:HA	5:B:623:HOH:O	1.95	0.66
1:B:53:GLN:HB3	5:B:623:HOH:O	1.96	0.66
1:A:334:LEU:H	1:A:359:ASN:HD21	1.44	0.64
1:B:336:SER:OG	1:B:353:PRO:O	2.14	0.64
1:B:5:ARG:HB3	5:B:672:HOH:O	1.98	0.62
1:B:82:PHE:HE2	1:B:208:LEU:HD11	1.65	0.61
1:A:158:HIS:HD2	1:A:160:TRP:H	1.49	0.61
1:B:242:GLN:HE21	1:B:246:ARG:HE	1.49	0.60
1:A:257:GLU:OE1	1:B:222:ARG:CZ	2.53	0.57
1:B:30:TYR:HD1	5:B:660:HOH:O	1.87	0.56
1:A:82:PHE:HE1	1:A:208:LEU:HD11	1.69	0.56
1:B:211:LEU:O	1:B:211:LEU:HD23	2.06	0.56
1:B:5:ARG:C	5:B:672:HOH:O	2.50	0.55
1:B:182:LEU:HB3	5:B:704:HOH:O	2.07	0.54
1:B:48:TRP:CH2	1:B:123:ARG:HG3	2.43	0.54
1:A:41:LEU:O	1:A:44:THR:OG1	2.21	0.53
1:B:331:ARG:CD	1:B:331:ARG:C	2.80	0.53
1:A:364:GLU:HG2	5:A:732:HOH:O	2.08	0.52
1:B:13:GLN:HB3	5:B:620:HOH:O	2.09	0.52
1:B:211:LEU:HD23	1:B:211:LEU:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ASP:HA	5:B:707:HOH:O	2.09	0.51
1:B:82:PHE:HB2	1:B:188:ARG:HD2	1.93	0.51
1:B:383:LEU:O	1:B:387:GLU:HG2	2.11	0.51
1:B:331:ARG:HG3	1:B:332:TYR:CD2	2.46	0.51
1:B:357:ASN:HA	1:B:414:LEU:CD1	2.41	0.51
1:A:179:VAL:HG11	1:A:206:ARG:HD2	1.93	0.50
1:A:211:LEU:C	1:A:211:LEU:HD23	2.36	0.50
1:A:211:LEU:HD23	1:A:211:LEU:O	2.12	0.50
1:B:117:LYS:O	1:B:118:ASP:C	2.56	0.49
1:A:202:GLU:O	1:A:206:ARG:HD3	2.13	0.48
1:A:5:ARG:HH22	1:A:45:GLN:HE21	1.62	0.48
1:A:82:PHE:CE1	1:A:208:LEU:HD11	2.48	0.48
1:B:278:ASP:OD2	1:B:285:PHE:HE2	1.97	0.48
1:B:5:ARG:CB	5:B:672:HOH:O	2.59	0.48
1:B:82:PHE:CZ	1:B:185:TYR:HB2	2.49	0.47
1:A:176:ARG:NH2	1:A:288:ASP:OD2	2.47	0.47
1:A:383:LEU:O	1:A:387:GLU:HG2	2.15	0.46
1:B:160:TRP:CD1	4:B:502:DGY:H3C1	2.51	0.45
1:A:204:TYR:HA	1:A:207:TYR:CD2	2.51	0.45
1:B:350:TRP:CE2	1:B:355:TRP:CZ2	3.05	0.45
1:B:113:TYR:CE1	1:B:117:LYS:HG3	2.51	0.45
1:B:5:ARG:HH22	1:B:45:GLN:HE21	1.66	0.44
1:A:357:ASN:HA	1:A:414:LEU:CD1	2.48	0.43
1:A:337:VAL:O	1:A:338:ASP:C	2.62	0.43
1:B:165:ASP:CB	5:B:705:HOH:O	2.57	0.43
1:B:204:TYR:HA	1:B:207:TYR:CD2	2.52	0.43
1:B:48:TRP:CD1	5:B:708:HOH:O	2.72	0.43
1:A:113:TYR:CE1	1:A:117:LYS:HG3	2.54	0.43
1:B:337:VAL:O	1:B:338:ASP:C	2.61	0.43
1:B:33:LEU:C	1:B:33:LEU:HD23	2.44	0.42
1:B:41:LEU:O	1:B:44:THR:OG1	2.20	0.42
1:B:47:ASP:HA	5:B:674:HOH:O	2.18	0.42
1:B:331:ARG:C	1:B:331:ARG:HD2	2.45	0.42
1:B:393:GLU:HG3	1:B:408:PHE:CE1	2.54	0.42
1:B:45:GLN:HB2	1:B:416:LEU:HD23	2.01	0.42
1:B:170:TRP:CZ3	1:B:232:VAL:HG11	2.55	0.42
1:B:172:LYS:NZ	1:B:293:GLU:OE1	2.53	0.42
1:B:48:TRP:CE3	1:B:49:GLU:N	2.89	0.41
1:A:77:GLN:NE2	5:A:724:HOH:O	2.54	0.41
1:B:71:HIS:HB2	1:B:103:GLN:HG3	2.01	0.41
1:B:35:ASP:HA	1:B:410:TRP:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TRP:CE2	1:B:72:ILE:HG12	2.56	0.40
1:B:410:TRP:CD1	1:B:410:TRP:C	2.98	0.40
1:A:32:TRP:CE2	1:A:72:ILE:HG12	2.57	0.40
1:A:28:TYR:CZ	3:A:501:TRS:H21	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:633:HOH:O	5:B:633:HOH:O[2_655]	0.70	1.50

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	409/420 (97%)	395 (97%)	13 (3%)	1 (0%)	43	44
1	B	405/420 (96%)	390 (96%)	14 (4%)	1 (0%)	43	44
All	All	814/840 (97%)	785 (96%)	27 (3%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	349	TYR
1	A	349	TYR

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	345/349 (99%)	336 (97%)	9 (3%)	40	46
1	B	342/349 (98%)	335 (98%)	7 (2%)	48	56
All	All	687/698 (98%)	671 (98%)	16 (2%)	44	51

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	150	ARG
1	A	186	GLU
1	A	256	GLN
1	A	276	LEU
1	A	317	SER
1	A	336	SER
1	A	349	TYR
1	A	410	TRP
1	B	71	HIS
1	B	114	LEU
1	B	256	GLN
1	B	331	ARG
1	B	336	SER
1	B	349	TYR
1	B	410	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	75	HIS
1	A	77	GLN
1	A	158	HIS
1	A	192	HIS
1	A	227	GLN
1	A	321	GLN
1	A	359	ASN
1	B	45	GLN
1	B	75	HIS
1	B	227	GLN

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Mol	Chain	Res	Type
1	B	242	GLN
1	B	245	ASN
1	B	321	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	TRS	B	501	-	7,7,7	0.49	0	9,9,9	0.21	0
4	DGY	A	502	-	6,6,6	1.01	0	6,7,7	1.79	2 (33%)
3	TRS	A	501	-	7,7,7	0.91	0	9,9,9	4.23	7 (77%)
4	DGY	B	502	-	6,6,6	0.91	0	6,7,7	1.89	1 (16%)

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	TRS	B	501	-	-	6/9/9/9	-
4	DGY	A	502	-	-	5/6/6/6	-
3	TRS	A	501	-	-	5/9/9/9	-
4	DGY	B	502	-	-	1/6/6/6	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	TRS	C2-C-N	-6.06	92.72	108.17
3	A	501	TRS	C1-C-N	-5.25	94.77	108.17
3	A	501	TRS	C3-C-N	-5.17	94.99	108.17
3	A	501	TRS	C3-C-C2	4.54	122.74	110.66
3	A	501	TRS	C2-C-C1	4.50	122.65	110.66
3	A	501	TRS	O1-C1-C	-3.97	99.82	110.88
4	B	502	DGY	O1-C1-C2	3.75	120.66	112.74
4	A	502	DGY	O2-C1-C2	-3.14	116.33	122.60
3	A	501	TRS	O2-C2-C	-3.00	102.50	110.88
4	A	502	DGY	O1-C1-C2	2.90	118.88	112.74

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	TRS	C2-C-C1-O1
3	A	501	TRS	C2-C-C3-O3
4	A	502	DGY	O1-C1-C2-C3
3	B	501	TRS	C1-C-C2-O2
4	A	502	DGY	O2-C1-C2-C3
4	B	502	DGY	C1-C2-C3-O4
3	A	501	TRS	N-C-C1-O1
3	A	501	TRS	C1-C-C2-O2
3	B	501	TRS	N-C-C2-O2
3	B	501	TRS	N-C-C3-O3
3	B	501	TRS	C3-C-C2-O2
3	B	501	TRS	C1-C-C3-O3
3	B	501	TRS	C2-C-C3-O3
4	A	502	DGY	O3-C2-C3-O4
4	A	502	DGY	O1-C1-C2-O3
4	A	502	DGY	O2-C1-C2-O3
3	A	501	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	TRS	1	0
4	B	502	DGY	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

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	413/420 (98%)	0.57	22 (5%) 32 34	14, 23, 39, 54	0
1	B	409/420 (97%)	2.31	227 (55%) 0 0	18, 35, 54, 69	0
All	All	822/840 (97%)	1.44	249 (30%) 1 1	14, 28, 49, 69	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	TRP	9.5
1	B	212	TYR	7.4
1	B	398	LEU	7.3
1	B	184	PRO	6.2
1	B	397	PRO	6.0
1	B	402	GLY	5.8
1	B	390	GLY	5.7
1	B	160	TRP	5.6
1	B	3	PRO	5.6
1	B	12	LEU	5.5
1	B	219	TYR	5.5
1	B	337	VAL	5.4
1	B	331	ARG	5.2
1	B	394	TYR	5.2
1	B	22	VAL	5.2
1	B	201	LYS	5.2
1	B	208	LEU	5.1
1	B	211	LEU	5.1
1	B	20	PHE	5.1
1	B	75	HIS	5.0
1	B	43	TRP	4.9
1	B	407	GLY	4.9
1	B	81	TYR	4.9
1	B	51	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	330	ALA	4.8
1	B	408	PHE	4.8
1	B	73	VAL	4.8
1	B	193	VAL	4.8
1	B	123	ARG	4.7
1	B	24	ALA	4.7
1	B	124	ALA	4.6
1	B	385	LEU	4.6
1	B	46	VAL	4.6
1	B	199	PRO	4.5
1	B	339	PRO	4.5
1	B	401	GLN	4.5
1	B	96	PRO	4.5
1	B	174	LEU	4.4
1	B	207	TYR	4.4
1	B	30	TYR	4.4
1	B	396	ASP	4.4
1	B	78	SER	4.4
1	B	173	PRO	4.3
1	B	9	VAL	4.2
1	B	403	ARG	4.2
1	B	224	ILE	4.2
1	B	37	ALA	4.2
1	B	203	ASP	4.1
1	B	388	ARG	4.1
1	B	4	LEU	4.1
1	B	77	GLN	4.0
1	B	214	PHE	4.0
1	B	332	TYR	4.0
1	B	97	ALA	3.9
1	B	181	ASN	3.9
1	B	329	LYS	3.9
1	B	202	GLU	3.9
1	B	47	ASP	3.9
1	B	26	GLY	3.9
1	B	210	LEU	3.9
1	B	11	VAL	3.9
1	B	354	VAL	3.9
1	B	344	PHE	3.9
1	B	405	GLY	3.9
1	B	348	ARG	3.9
1	B	178	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	32	TRP	3.8
1	B	409	SER	3.8
1	B	8	ALA	3.8
1	B	230	PHE	3.8
1	A	76	GLU	3.8
1	A	77	GLN	3.8
1	B	415	ALA	3.7
1	B	176	ARG	3.7
1	B	187	ARG	3.7
1	B	414	LEU	3.7
1	B	290	VAL	3.7
1	B	215	ARG	3.7
1	B	179	VAL	3.6
1	B	18	GLY	3.6
1	B	404	GLY	3.6
1	B	98	THR	3.6
1	A	222	ARG	3.6
1	B	52	TRP	3.5
1	B	182	LEU	3.5
1	B	327	GLY	3.5
1	B	349	TYR	3.5
1	B	82	PHE	3.5
1	B	83	PRO	3.5
1	B	227	GLN	3.5
1	B	399	THR	3.5
1	B	323	ALA	3.5
1	B	343	PHE	3.4
1	B	341	SER	3.4
1	B	80	ASP	3.4
1	B	76	GLU	3.4
1	B	61	TYR	3.4
1	B	79	ARG	3.4
1	B	118	ASP	3.4
1	B	40	ALA	3.4
1	B	389	GLU	3.4
1	B	383	LEU	3.4
1	B	340	THR	3.4
1	B	395	TYR	3.4
1	B	198	ARG	3.4
1	B	195	PRO	3.4
1	B	229	PRO	3.4
1	B	400	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	19	ALA	3.4
1	B	21	THR	3.3
1	B	228	SER	3.3
1	B	356	ILE	3.3
1	B	200	ARG	3.3
1	B	206	ARG	3.3
1	B	190	VAL	3.3
1	B	169	ALA	3.3
1	B	177	VAL	3.2
1	B	180	GLU	3.2
1	B	55	LEU	3.2
1	B	172	LYS	3.2
1	B	85	PRO	3.2
1	B	125	ARG	3.2
1	B	222	ARG	3.2
1	B	416	LEU	3.2
1	B	167	SER	3.2
1	B	386	MET	3.2
1	B	71	HIS	3.1
1	B	122	ASP	3.1
1	B	382	ALA	3.1
1	B	217	LEU	3.1
1	B	204	TYR	3.1
1	B	158	HIS	3.1
1	B	113	TYR	3.0
1	A	3	PRO	3.0
1	B	197	GLU	3.0
1	B	157	VAL	3.0
1	B	166	ASN	3.0
1	B	412	ALA	3.0
1	B	33	LEU	3.0
1	B	34	TRP	3.0
1	B	392	ARG	2.9
1	B	333	LEU	2.9
1	B	39	ILE	2.9
1	B	391	PHE	2.9
1	B	72	ILE	2.9
1	B	185	TYR	2.9
1	B	355	TRP	2.9
1	A	182	LEU	2.9
1	B	183	PRO	2.9
1	B	120	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	2.8
1	B	29	PRO	2.8
1	B	16	SER	2.8
1	B	175	SER	2.8
1	A	86	ASP	2.8
1	B	347	GLY	2.8
1	B	56	LEU	2.8
1	A	183	PRO	2.8
1	B	49	GLU	2.8
1	B	84	GLY	2.8
1	B	384	ALA	2.8
1	B	27	LEU	2.8
1	B	342	PRO	2.8
1	B	15	ASN	2.7
1	B	225	TYR	2.7
1	B	419	THR	2.7
1	B	58	LEU	2.7
1	B	159	PRO	2.7
1	B	410	TRP	2.7
1	B	352	GLY	2.7
1	B	351	ARG	2.7
1	B	45	GLN	2.7
1	B	59	PHE	2.7
1	B	74	PHE	2.7
1	B	128	ALA	2.7
1	B	23	PRO	2.7
1	B	387	GLU	2.7
1	B	127	ARG	2.6
1	B	226	ARG	2.6
1	B	168	PRO	2.6
1	B	171	ASP	2.6
1	B	231	LYS	2.6
1	A	84	GLY	2.6
1	B	196	GLU	2.6
1	B	141	TRP	2.6
1	B	350	TRP	2.6
1	B	413	ALA	2.6
1	B	69	LEU	2.6
1	B	345	GLU	2.6
1	B	100	GLY	2.6
1	B	60	ASP	2.6
1	B	129	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	38	PHE	2.5
1	B	13	GLN	2.5
1	A	226	ARG	2.5
1	B	28	TYR	2.5
1	B	41	LEU	2.5
1	B	150	ARG	2.5
1	B	86	ASP	2.4
1	B	70	PRO	2.4
1	A	14	ARG	2.4
1	B	326	TRP	2.4
1	B	6	THR	2.4
1	B	156	ILE	2.4
1	B	192	HIS	2.4
1	A	180	GLU	2.4
1	B	194	ASN	2.4
1	B	367	ARG	2.4
1	B	119	PRO	2.4
1	B	353	PRO	2.4
1	B	406	GLU	2.3
1	A	179	VAL	2.3
1	B	393	GLU	2.3
1	B	170	TRP	2.3
1	B	376	ALA	2.3
1	B	380	ALA	2.3
1	B	132	PHE	2.3
1	A	224	ILE	2.3
1	B	44	THR	2.3
1	B	42	GLY	2.3
1	B	328	GLU	2.3
1	B	111	VAL	2.3
1	B	221	PRO	2.3
1	B	357	ASN	2.3
1	B	281	ALA	2.3
1	A	96	PRO	2.2
1	A	79	ARG	2.2
1	B	189	ASP	2.2
1	B	50	ARG	2.2
1	B	295	ILE	2.2
1	A	219	TYR	2.2
1	A	129	ARG	2.2
1	A	367	ARG	2.2
1	B	364	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	ARG	2.2
1	A	191	LYS	2.2
1	B	358	VAL	2.1
1	B	291	ALA	2.1
1	B	191	LYS	2.1
1	B	418	TRP	2.1
1	A	217	LEU	2.1
1	B	126	GLU	2.1
1	A	90	ARG	2.1
1	B	5	ARG	2.1
1	A	172	LYS	2.1
1	B	411	SER	2.1
1	B	57	CYS	2.0
1	B	14	ARG	2.0
1	B	130	TYR	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
4	DGY	B	502	7/7	0.77	0.20	28,31,35,36	0
3	TRS	B	501	8/8	0.82	0.19	30,35,38,40	0
3	TRS	A	501	8/8	0.86	0.16	32,36,38,40	0
4	DGY	A	502	7/7	0.93	0.10	19,19,21,21	0
2	CL	B	500	1/1	0.99	0.02	20,20,20,20	1
2	CL	A	500	1/1	1.00	0.02	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.