



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 PM UTC

PDB ID : 1GVF / pdb_00001gvf
Title : Structure of tagatose-1,6-bisphosphate aldolase
Authors : Hall, D.R.; Hunter, W.N.
Deposited on : 2002-02-11
Resolution : 1.45 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

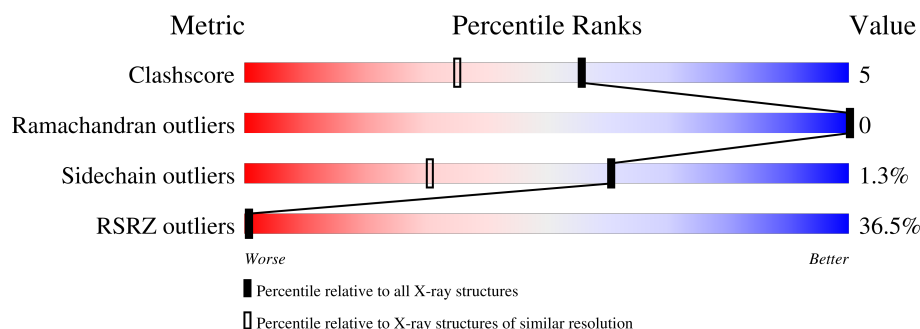
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	286	33% 86% 8% • 5%
1	B	286	37% 84% 11% • •

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	PGH	B	287	-	X	-	-
5	EDO	B	1294	-	X	X	-

2 Entry composition [i](#)

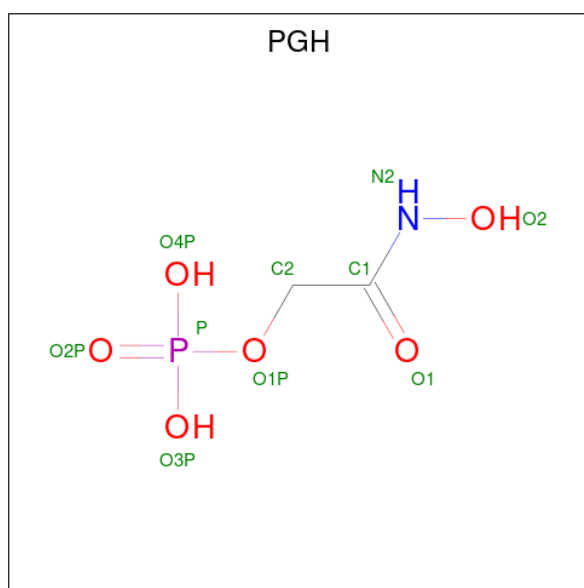
There are 6 unique types of molecules in this entry. The entry contains 4997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TAGATOSE-BISPHOSPHATE ALDOLASE AGAY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	7	0
			2115	1339	368	397	11			
1	B	275	Total	C	N	O	S	0	8	0
			2144	1359	380	394	11			

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: $C_2H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

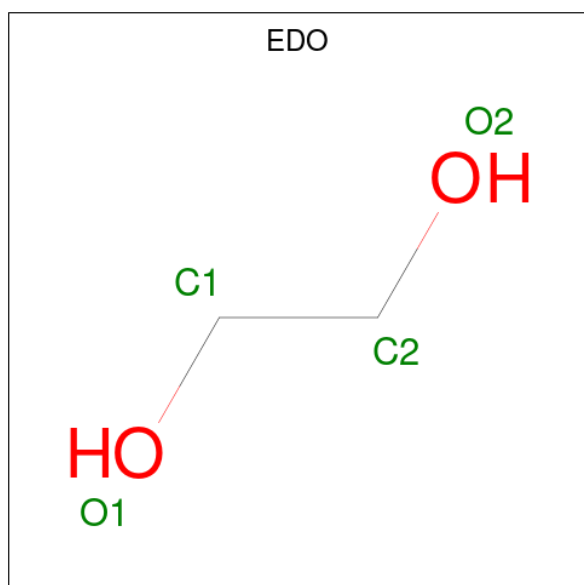
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

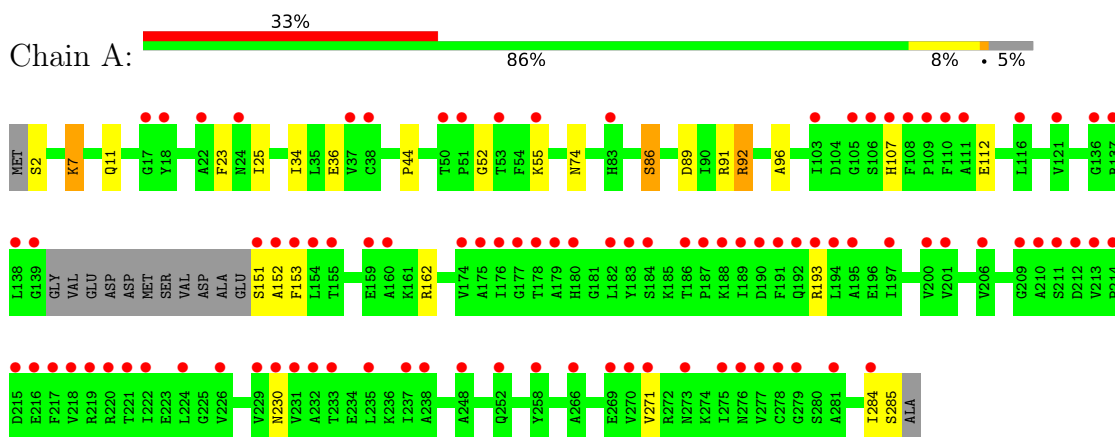
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	353	Total O 353 353	0	2
6	B	305	Total O 305 305	0	1

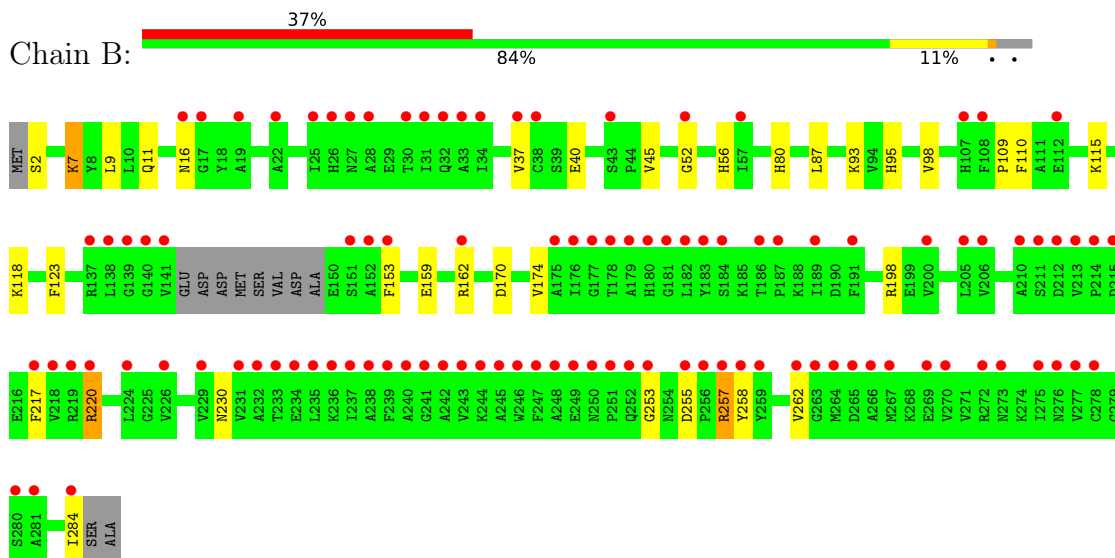
3 Residue-property plots [i](#)

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: TAGATOSE-BISPHOSPHATE ALDOLASE AGAY



• Molecule 1: TAGATOSE-BISPHOSPHATE ALDOLASE AGAY



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	72.65Å 100.46Å 206.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.45 10.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	93.4 (10.00-1.45) 90.3 (10.00-2.17)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.18Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.127 , 0.173 0.272 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4997	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: EDO, NA, ZN, PGH

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	0.78	0/2188	1.34	14/2970 (0.5%)
1	B	0.76	0/2216	1.47	19/3005 (0.6%)
All	All	0.77	0/4404	1.41	33/5975 (0.6%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	ARG	CD-NE-CZ	14.51	144.72	124.40
1	A	52	GLY	CA-C-N	8.25	131.67	120.54
1	A	52	GLY	C-N-CA	8.25	131.67	120.54
1	B	56	HIS	CA-CB-CG	7.55	121.35	113.80
1	A	92	ARG	CD-NE-CZ	7.43	134.81	124.40
1	A	107	HIS	CA-CB-CG	-7.23	106.57	113.80
1	A	151	SER	CA-C-N	7.21	132.76	120.72
1	A	151	SER	C-N-CA	7.21	132.76	120.72
1	A	153	PHE	CA-CB-CG	-7.19	106.61	113.80
1	B	220	ARG	NH1-CZ-NH2	6.49	127.74	119.30
1	A	11	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	B	87	LEU	CA-C-O	-6.05	114.14	120.55
1	B	174	VAL	CA-C-O	5.93	128.58	121.93
1	B	11	GLN	OE1-CD-NE2	-5.88	116.72	122.60
1	A	230	ASN	CA-CB-CG	5.80	118.40	112.60
1	B	262	VAL	O-C-N	-5.62	116.41	121.87
1	B	230	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	52	GLY	CA-C-N	5.50	127.96	120.54
1	B	52	GLY	C-N-CA	5.50	127.96	120.54
1	A	7	LYS	CA-CB-CG	5.47	125.05	114.10
1	A	86	SER	CA-CB-OG	5.47	122.05	111.10
1	A	152	ALA	N-CA-C	-5.46	105.89	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	174	VAL	CA-C-N	5.29	131.12	123.13
1	B	174	VAL	C-N-CA	5.29	131.12	123.13
1	B	153	PHE	CA-CB-CG	-5.25	108.56	113.80
1	B	217	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	253	GLY	CA-C-O	-5.16	116.33	121.90
1	A	285	SER	CA-C-O	-5.05	112.21	120.80
1	B	153	PHE	CA-C-N	-5.04	113.86	122.33
1	B	153	PHE	C-N-CA	-5.04	113.86	122.33
1	A	25	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	B	80	HIS	CA-CB-CG	5.01	118.81	113.80

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	2115	0	2084	17	0
1	B	2144	0	2139	22	0
2	A	10	0	3	0	0
2	B	10	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	36	7	0
5	B	32	0	48	12	0
6	A	353	0	0	4	0
6	B	305	0	0	9	0
All	All	4997	0	4313	41	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 5.

All (41) 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)
5:B:1294:EDO:C2	5:B:1294:EDO:C1	2.41	0.98
1:A:7:LYS:HG2	6:B:2151:HOH:O	1.87	0.75
1:A:193:ARG:HB2	5:A:1291:EDO:H11	1.71	0.73
1:A:7:LYS:HD3	6:B:2010:HOH:O	1.88	0.73
5:B:1294:EDO:H22	6:B:2140:HOH:O	1.95	0.67
1:A:112:GLU:HG2	6:A:2187:HOH:O	1.96	0.65
1:A:284:ILE:HG22	5:A:1294:EDO:H21	1.82	0.62
1:A:74:ASN:OD1	5:B:1292:EDO:H22	2.04	0.58
1:A:96:ALA:O	5:A:1293:EDO:H11	2.05	0.56
1:B:115:LYS:HA	5:B:1294:EDO:H11	1.88	0.55
1:B:37:VAL:O	1:B:40:GLU:HG3	2.07	0.55
1:B:255:ASP:HB3	1:B:258:TYR:CD2	2.43	0.54
1:B:7[B]:LYS:HD3	1:B:170:ASP:OD1	2.08	0.53
1:A:2:SER:N	5:A:1289:EDO:HO1	2.05	0.53
1:B:95:HIS:CE1	5:B:1292:EDO:H11	2.43	0.52
1:B:115:LYS:HB2	5:B:1294:EDO:H11	1.90	0.52
1:B:109:PRO:HB2	6:B:2137:HOH:O	2.10	0.52
1:B:115:LYS:CA	5:B:1294:EDO:H11	2.39	0.52
6:A:2014:HOH:O	1:B:7[A]:LYS:HE3	2.10	0.52
1:B:198[B]:ARG:HD2	6:B:2209:HOH:O	2.09	0.51
1:A:162:ARG:HD2	6:A:2221:HOH:O	2.10	0.51
1:A:36:GLU:OE2	5:A:1292:EDO:H11	2.11	0.50
1:B:115:LYS:CB	5:B:1294:EDO:H11	2.43	0.49
1:B:45:VAL:H	5:B:1288:EDO:H22	1.77	0.48
1:B:7[B]:LYS:HE3	6:B:2183:HOH:O	2.14	0.48
1:B:118:LYS:HD3	5:B:1294:EDO:C2	2.44	0.47
1:B:2:SER:N	5:B:1289:EDO:HO1	2.11	0.47
1:B:93:LYS:O	1:B:98[B]:VAL:HG22	2.14	0.47
1:A:91[B]:ARG:NH1	6:A:2147:HOH:O	2.49	0.44
1:A:36:GLU:OE2	5:A:1292:EDO:H22	2.17	0.44
1:B:110:PHE:CE1	1:B:159:GLU:HG2	2.53	0.44
1:B:220:ARG:NH2	6:B:2236:HOH:O	2.49	0.44
1:A:23:PHE:CG	1:A:34[B]:ILE:HD12	2.53	0.44
1:A:34[B]:ILE:HD13	1:A:271:VAL:CG2	2.48	0.44
1:A:89:ASP:OD1	1:A:92:ARG:NH2	2.51	0.43
1:B:7[A]:LYS:NZ	6:B:2007:HOH:O	2.51	0.42
1:B:9:LEU:HD12	6:B:2027:HOH:O	2.17	0.42
1:B:123:PHE:HB2	5:B:1295:EDO:H11	2.02	0.41
1:A:34[B]:ILE:HD13	1:A:271:VAL:HG21	2.03	0.41
1:A:44:PRO:HB3	5:A:1294:EDO:H11	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/286 (96%)	270 (98%)	6 (2%)	0	100	100
1	B	279/286 (98%)	273 (98%)	6 (2%)	0	100	100
All	All	555/572 (97%)	543 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	229/237 (97%)	227 (99%)	2 (1%)	70	46
1	B	231/237 (98%)	225 (97%)	6 (3%)	40	10
All	All	460/474 (97%)	452 (98%)	8 (2%)	61	21

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	86	SER
1	B	7[A]	LYS
1	B	7[B]	LYS
1	B	162[A]	ARG
1	B	162[B]	ARG
1	B	257	ARG
1	B	284	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	113	ASN
1	A	282	ASN
1	B	56	HIS
1	B	282	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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	$\# Z > 2$
5	EDO	A	1293	-	3,3,3	0.75	0	2,2,2	0.66	0
5	EDO	B	1295	-	3,3,3	0.51	0	2,2,2	0.30	0
5	EDO	B	1288	-	3,3,3	0.67	0	2,2,2	0.48	0
2	PGH	A	287	4,3	9,9,9	4.68	4 (44%)	10,12,12	3.85	3 (30%)
5	EDO	A	1290	-	3,3,3	0.61	0	2,2,2	0.31	0
5	EDO	B	1291	-	3,3,3	0.72	0	2,2,2	0.51	0
5	EDO	B	1293	-	3,3,3	0.64	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1289	-	3,3,3	0.77	0	2,2,2	1.11	0
5	EDO	A	1291	-	3,3,3	0.56	0	2,2,2	0.85	0
5	EDO	A	1292	-	3,3,3	0.70	0	2,2,2	0.29	0
2	PGH	B	287	4,3	9,9,9	3.67	5 (55%)	10,12,12	2.69	5 (50%)
5	EDO	B	1289	-	3,3,3	0.56	0	2,2,2	0.68	0
5	EDO	A	1294	-	3,3,3	0.57	0	2,2,2	0.57	0
5	EDO	B	1294	-	3,3,3	6.83	1 (33%)	2,2,2	3.41	2 (100%)
5	EDO	B	1290	-	3,3,3	0.30	0	2,2,2	0.37	0
5	EDO	B	1292	-	3,3,3	0.64	0	2,2,2	0.32	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
5	EDO	A	1293	-	-	1/1/1/1	-
5	EDO	B	1295	-	-	1/1/1/1	-
5	EDO	B	1288	-	-	0/1/1/1	-
2	PGH	A	287	4,3	-	4/8/8/8	-
5	EDO	A	1290	-	-	1/1/1/1	-
5	EDO	B	1291	-	-	0/1/1/1	-
5	EDO	B	1293	-	-	1/1/1/1	-
5	EDO	A	1289	-	-	0/1/1/1	-
5	EDO	A	1291	-	-	1/1/1/1	-
5	EDO	A	1292	-	-	1/1/1/1	-
2	PGH	B	287	4,3	-	3/8/8/8	-
5	EDO	B	1289	-	-	0/1/1/1	-
5	EDO	A	1294	-	-	0/1/1/1	-
5	EDO	B	1294	-	-	1/1/1/1	-
5	EDO	B	1290	-	-	1/1/1/1	-
5	EDO	B	1292	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1294	EDO	C2-C1	11.82	2.41	1.48
2	A	287	PGH	O1P-C2	9.75	1.53	1.43
2	A	287	PGH	C2-C1	9.43	1.70	1.51
2	B	287	PGH	C2-C1	7.06	1.65	1.51
2	B	287	PGH	C1-N2	6.44	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	PGH	P-O3P	-3.47	1.41	1.54
2	B	287	PGH	O2-N2	2.88	1.46	1.40
2	B	287	PGH	P-O2P	-2.35	1.43	1.50
2	A	287	PGH	O2-N2	2.09	1.45	1.40
2	A	287	PGH	C1-N2	-2.03	1.30	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	287	PGH	O2-N2-C1	-7.40	108.86	119.79
2	A	287	PGH	O1-C1-N2	6.78	131.59	123.27
2	A	287	PGH	C2-C1-N2	-6.40	105.38	116.41
2	B	287	PGH	C2-C1-N2	-5.23	107.41	116.41
2	B	287	PGH	O1-C1-C2	4.72	132.63	119.65
5	B	1294	EDO	O2-C2-C1	-3.49	85.85	112.39
2	B	287	PGH	O1-C1-N2	-3.34	119.17	123.27
5	B	1294	EDO	O1-C1-C2	-3.32	87.08	112.39
2	B	287	PGH	O4P-P-O3P	2.29	116.37	107.80
2	B	287	PGH	O2-N2-C1	-2.03	116.80	119.79

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	287	PGH	C2-O1P-P-O2P
2	A	287	PGH	C2-O1P-P-O3P
2	A	287	PGH	C2-O1P-P-O4P
2	B	287	PGH	C2-O1P-P-O3P
5	A	1293	EDO	O1-C1-C2-O2
5	B	1290	EDO	O1-C1-C2-O2
5	B	1294	EDO	O1-C1-C2-O2
5	B	1295	EDO	O1-C1-C2-O2
2	B	287	PGH	C2-O1P-P-O4P
2	B	287	PGH	O1-C1-C2-O1P
2	A	287	PGH	O1-C1-C2-O1P
5	A	1292	EDO	O1-C1-C2-O2
5	B	1292	EDO	O1-C1-C2-O2
5	B	1293	EDO	O1-C1-C2-O2
5	A	1291	EDO	O1-C1-C2-O2
5	A	1290	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1293	EDO	1	0
5	B	1295	EDO	1	0
5	B	1288	EDO	1	0
5	A	1289	EDO	1	0
5	A	1291	EDO	1	0
5	A	1292	EDO	2	0
5	B	1289	EDO	1	0
5	A	1294	EDO	2	0
5	B	1294	EDO	7	0
5	B	1292	EDO	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

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	273/286 (95%)	1.80	95 (34%)  	10, 15, 33, 56	7 (2%)
1	B	275/286 (96%)	1.89	105 (38%)  	9, 18, 35, 54	8 (2%)
All	All	548/572 (95%)	1.84	200 (36%)  	9, 16, 34, 56	15 (2%)

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	8.8
1	B	246	TRP	8.2
1	A	184	SER	7.1
1	B	248	ALA	6.5
1	B	258	TYR	6.5
1	B	245	ALA	6.2
1	B	266	ALA	6.1
1	B	241	GLY	6.1
1	B	251	PRO	5.8
1	A	152	ALA	5.7
1	B	238	ALA	5.6
1	A	183	TYR	5.3
1	B	259	TYR	5.2
1	A	182	LEU	5.2
1	A	191	PHE	5.2
1	A	177	GLY	5.1
1	A	179	ALA	5.1
1	B	242	ALA	5.1
1	B	240	ALA	4.9
1	A	109	PRO	4.9
1	B	262	VAL	4.9
1	A	105	GLY	4.8
1	A	189	ILE	4.8
1	A	217	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	256	PRO	4.6
1	B	141	VAL	4.4
1	A	151	SER	4.4
1	B	239	PHE	4.4
1	B	179	ALA	4.3
1	A	154	LEU	4.2
1	A	214	PRO	4.2
1	A	190	ASP	4.1
1	A	210	ALA	4.1
1	A	216	GLU	4.1
1	B	177	GLY	4.1
1	A	220	ARG	4.0
1	B	237	ILE	4.0
1	B	249	GLU	4.0
1	A	107	HIS	4.0
1	B	37	VAL	4.0
1	A	176	ILE	4.0
1	B	247	PHE	3.9
1	B	263	GLY	3.9
1	A	138	LEU	3.9
1	A	108	PHE	3.9
1	A	213	VAL	3.8
1	A	231	VAL	3.8
1	A	211	SER	3.8
1	A	22	ALA	3.8
1	B	217	PHE	3.7
1	A	266	ALA	3.7
1	B	212	ASP	3.7
1	B	182	LEU	3.7
1	A	270	VAL	3.7
1	B	184	SER	3.7
1	A	273	ASN	3.7
1	B	233	THR	3.6
1	B	270	VAL	3.6
1	B	252	GLN	3.6
1	B	232	ALA	3.6
1	A	136	GLY	3.5
1	B	153	PHE	3.5
1	A	111	ALA	3.5
1	A	226	VAL	3.5
1	B	243	VAL	3.5
1	A	238	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	265	ASP	3.5
1	A	276	ASN	3.5
1	B	183	TYR	3.4
1	A	277	VAL	3.4
1	B	277[A]	VAL	3.4
1	B	33	ALA	3.4
1	B	236	LYS	3.3
1	A	187	PRO	3.3
1	A	186	THR	3.3
1	A	233	THR	3.3
1	A	258	TYR	3.3
1	A	51	PRO	3.3
1	A	224	LEU	3.3
1	A	197	ILE	3.3
1	A	278	CYS	3.2
1	A	137	ARG	3.2
1	A	222	ILE	3.2
1	B	26	HIS	3.2
1	A	178	THR	3.2
1	A	212	ASP	3.1
1	A	174	VAL	3.1
1	A	219	ARG	3.1
1	B	275	ILE	3.1
1	A	232	ALA	3.1
1	A	230	ASN	3.1
1	B	253	GLY	3.1
1	B	255	ASP	3.1
1	B	211	SER	3.0
1	A	53	THR	3.0
1	B	28	ALA	2.9
1	B	189	ILE	2.9
1	A	200	VAL	2.9
1	B	186	THR	2.9
1	B	52	GLY	2.9
1	A	194	LEU	2.8
1	B	214	PRO	2.8
1	B	137	ARG	2.8
1	B	213	VAL	2.8
1	A	83	HIS	2.8
1	A	17	GLY	2.8
1	B	140	GLY	2.8
1	A	284	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	284	ILE	2.8
1	A	271	VAL	2.7
1	B	231	VAL	2.7
1	B	235	LEU	2.7
1	B	269	GLU	2.7
1	B	244	LYS	2.7
1	A	275	ILE	2.7
1	B	34	ILE	2.7
1	B	215	ASP	2.7
1	B	25	ILE	2.7
1	A	155	THR	2.6
1	B	151	SER	2.6
1	B	180	HIS	2.6
1	A	24	ASN	2.6
1	B	250	ASN	2.6
1	A	37	VAL	2.6
1	A	229	VAL	2.6
1	B	229	VAL	2.6
1	A	160	ALA	2.5
1	A	159[A]	GLU	2.5
1	A	193	ARG	2.5
1	B	210	ALA	2.5
1	B	176	ILE	2.5
1	B	219	ARG	2.5
1	B	257	ARG	2.5
1	A	188	LYS	2.5
1	A	50	THR	2.5
1	B	276	ASN	2.5
1	B	273	ASN	2.5
1	B	19	ALA	2.4
1	B	22	ALA	2.4
1	A	55	LYS	2.4
1	B	138	LEU	2.4
1	B	191	PHE	2.4
1	A	195	ALA	2.4
1	B	175	ALA	2.4
1	A	279	GLY	2.4
1	B	234	GLU	2.4
1	B	108	PHE	2.4
1	A	281	ALA	2.4
1	B	264	MET	2.4
1	B	281	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	38	CYS	2.4
1	A	237	ILE	2.4
1	B	272[A]	ARG	2.4
1	A	175	ALA	2.3
1	B	220	ARG	2.3
1	B	187	PRO	2.3
1	B	112	GLU	2.3
1	B	162[A]	ARG	2.3
1	A	215	ASP	2.3
1	B	181	GLY	2.3
1	A	103	ILE	2.3
1	B	31	ILE	2.3
1	A	106	SER	2.3
1	A	252	GLN	2.2
1	A	110	PHE	2.2
1	B	218	VAL	2.2
1	B	280	SER	2.2
1	A	116	LEU	2.2
1	B	16	ASN	2.2
1	B	32	GLN	2.2
1	A	209	GLY	2.2
1	B	43	SER	2.2
1	A	18	TYR	2.2
1	A	221	THR	2.2
1	A	121	VAL	2.2
1	A	206	VAL	2.2
1	A	218	VAL	2.2
1	B	226	VAL	2.2
1	A	139	GLY	2.1
1	B	57[A]	ILE	2.1
1	B	30	THR	2.1
1	B	178	THR	2.1
1	A	269	GLU	2.1
1	B	152	ALA	2.1
1	B	38	CYS	2.1
1	A	201	VAL	2.1
1	B	27	ASN	2.1
1	B	224	LEU	2.1
1	B	200	VAL	2.0
1	B	206	VAL	2.0
1	B	205	LEU	2.0
1	A	192	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	267	MET	2.0
1	B	17	GLY	2.0
1	B	139	GLY	2.0
1	A	180	HIS	2.0
1	B	107	HIS	2.0
1	A	248	ALA	2.0
1	A	235	LEU	2.0
1	B	278	CYS	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
5	EDO	B	1293	4/4	0.38	0.26	48,50,55,57	0
5	EDO	B	1295	4/4	0.57	0.30	49,51,53,59	0
5	EDO	A	1291	4/4	0.59	0.20	50,51,56,70	0
4	NA	B	289	1/1	0.64	0.18	16,16,16,16	0
4	NA	A	289	1/1	0.65	0.26	15,15,15,15	0
5	EDO	B	1294	4/4	0.67	0.15	38,47,49,63	0
5	EDO	B	1291	4/4	0.69	0.15	26,34,35,38	0
5	EDO	A	1294	4/4	0.73	0.22	34,35,52,58	0
5	EDO	B	1289	4/4	0.74	0.18	26,33,35,40	0
5	EDO	A	1292	4/4	0.76	0.15	47,53,55,67	0
3	ZN	A	288	1/1	0.79	0.09	12,12,12,12	0
3	ZN	B	288	1/1	0.79	0.09	12,12,12,12	0
5	EDO	B	1288	4/4	0.80	0.11	24,32,35,40	0
5	EDO	B	1292	4/4	0.81	0.20	44,52,56,66	0
5	EDO	A	1293	4/4	0.81	0.18	35,44,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1290	4/4	0.84	0.11	20,22,27,27	0
2	PGH	A	287	10/10	0.84	0.16	14,16,19,26	0
5	EDO	A	1289	4/4	0.86	0.11	19,20,24,27	0
5	EDO	B	1290	4/4	0.87	0.13	38,40,41,57	0
2	PGH	B	287	10/10	0.88	0.13	14,15,20,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.