



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2020 – 11:23 am GMT

PDB ID : 6YAJ
Title : Split gene transketolase, inactive beta4 tetramer
Authors : Isupov, M.N.; Littlechild, J.A.; James, P.
Deposited on : 2020-03-12
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

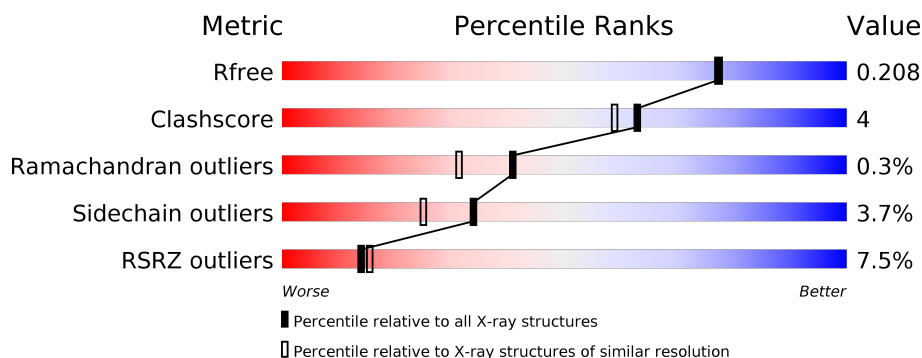
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	AAA	341	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
1	BBB	341	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>12%</div> </div> </div>
1	CCC	341	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>12%</div> </div> </div>
1	DDD	341	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	AAA	403	-	-	X	-
3	GOL	DDD	401	-	-	X	-

2 Entry composition [i](#)

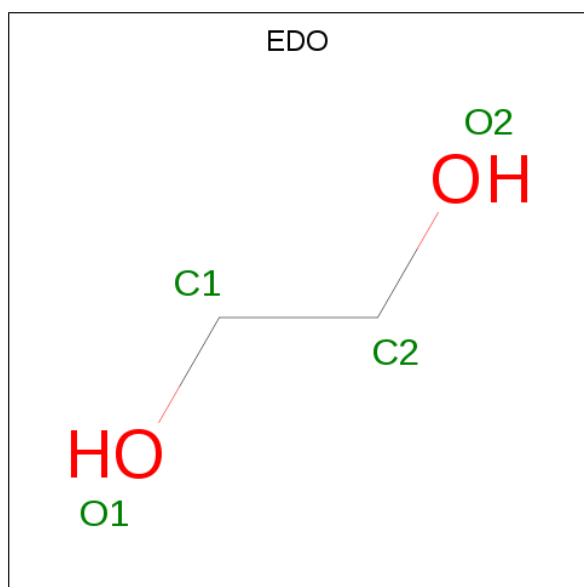
There are 5 unique types of molecules in this entry. The entry contains 9891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C-terminal chain of split transketolase from Carboxydothemus hydrogenoformans.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	303	Total	C	N	O	S	0	23	0
			2390	1533	410	438	9			
1	BBB	299	Total	C	N	O	S	0	17	0
			2305	1479	391	426	9			
1	CCC	300	Total	C	N	O	S	0	22	0
			2344	1507	393	436	8			
1	DDD	311	Total	C	N	O	S	0	20	0
			2415	1548	412	447	8			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	CCC	1	Total 4	C 2	O 2	0	0
2	CCC	1	Total 4	C 2	O 2	0	0
2	CCC	1	Total 4	C 2	O 2	0	0
2	DDD	1	Total 4	C 2	O 2	0	0
2	DDD	1	Total 4	C 2	O 2	0	0
2	DDD	1	Total 4	C 2	O 2	0	0
2	DDD	1	Total 4	C 2	O 2	0	0
2	DDD	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		
3	DDD	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

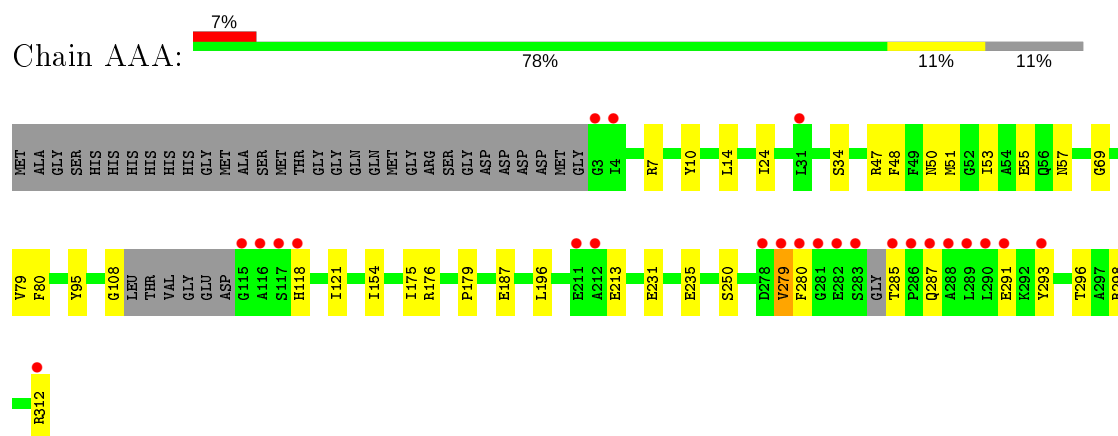
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	91	Total	O	0	0
			91	91		
5	BBB	81	Total	O	0	0
			81	81		
5	CCC	66	Total	O	0	0
			66	66		
5	DDD	96	Total	O	0	0
			96	96		

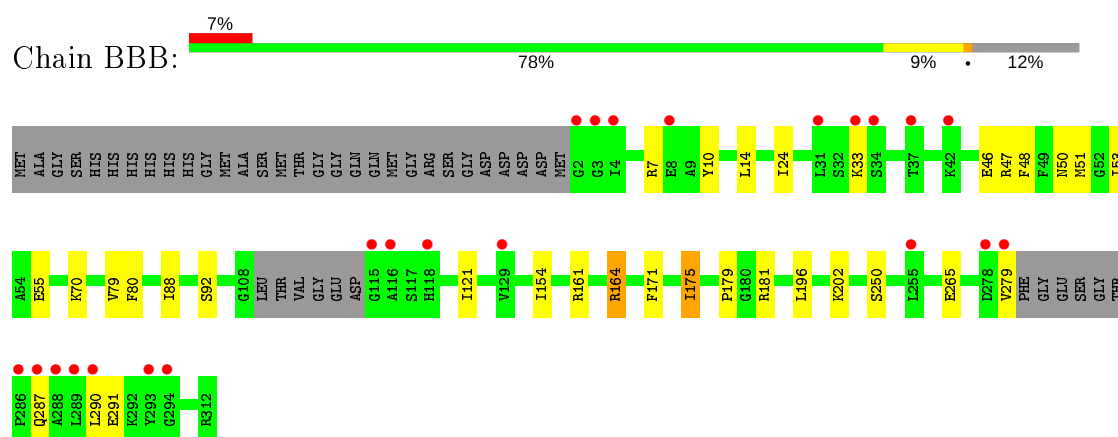
3 Residue-property plots

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.

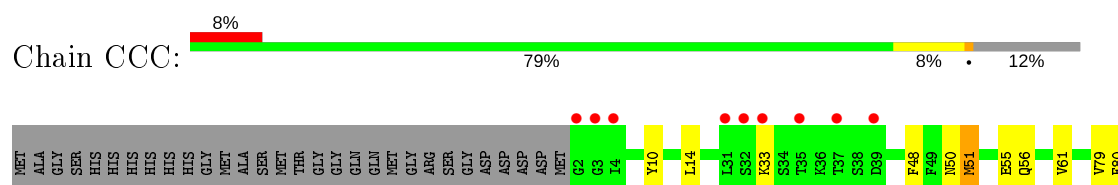
- Molecule 1: C-terminal chain of split transketolase from *Carboxydotherrmus hydrogenofor-*
mans

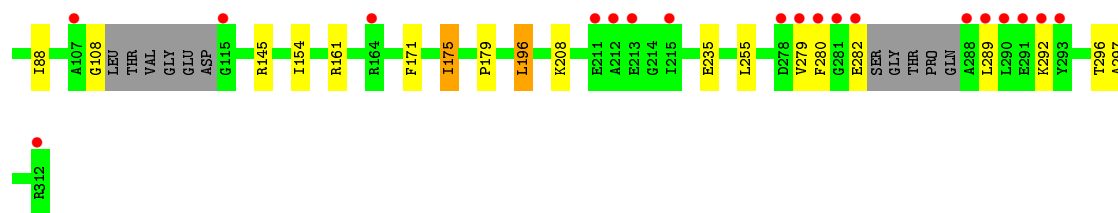


- Molecule 1: C-terminal chain of split transketolase from *Carboxydotherrmus hydrogenofor-*
mans

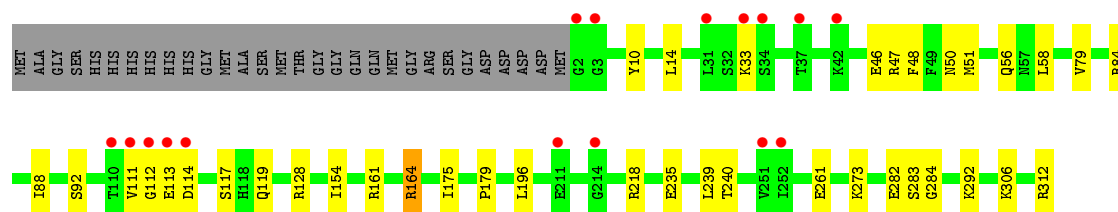
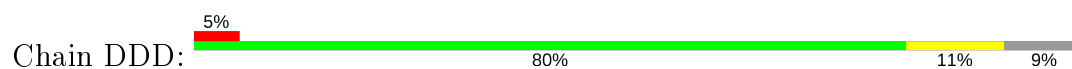


- Molecule 1: C-terminal chain of split transketolase from *Carboxydotherrmus hydrogenofor-*
mans





- Molecule 1: C-terminal chain of split transketolase from *Carboxydothermus hydrogenoformans*



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.88Å 101.88Å 164.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.01 – 1.90 64.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.01-1.90) 99.8 (64.01-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.208 0.178 , 0.208	Depositor DCC
R_{free} test set	6613 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9891	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GOL, PEG, EDO

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	AAA	0.54	3/2485 (0.1%)	0.78	0/3352
1	BBB	0.46	0/2387	0.78	3/3225 (0.1%)
1	CCC	0.48	2/2441 (0.1%)	0.76	0/3295
1	DDD	0.47	1/2509 (0.0%)	0.76	2/3391 (0.1%)
All	All	0.49	6/9822 (0.1%)	0.77	5/13263 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	213	GLU	CD-OE1	9.11	1.35	1.25
1	AAA	235	GLU	CD-OE1	7.68	1.34	1.25
1	CCC	235	GLU	CD-OE1	7.22	1.33	1.25
1	AAA	187	GLU	CD-OE1	6.37	1.32	1.25
1	CCC	235	GLU	CD-OE2	5.32	1.31	1.25
1	DDD	235	GLU	CD-OE1	5.06	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	181	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	BBB	7	ARG	CB-CG-CD	6.25	127.86	111.60
1	DDD	84	ARG	CG-CD-NE	5.64	123.64	111.80
1	BBB	7	ARG	CG-CD-NE	5.64	123.64	111.80
1	DDD	218	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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	AAA	2390	0	2549	22	0
1	BBB	2305	0	2449	23	0
1	CCC	2344	0	2492	20	0
1	DDD	2415	0	2569	24	0
2	AAA	16	0	24	1	0
2	BBB	12	0	18	1	0
2	CCC	12	0	18	2	0
2	DDD	20	0	30	1	0
3	AAA	6	0	8	4	0
3	BBB	12	0	16	2	0
3	CCC	6	0	8	3	0
3	DDD	12	0	16	4	0
4	BBB	7	0	10	0	0
5	AAA	91	0	0	3	0
5	BBB	81	0	0	1	0
5	CCC	66	0	0	0	0
5	DDD	96	0	0	5	0
All	All	9891	0	10207	85	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 (85) 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:AAA:296:THR:HB	3:AAA:403:GOL:H12	1.03	1.02
1:DDD:46:GLU:HB2	3:DDD:401:GOL:H12	1.39	1.01
1:AAA:296:THR:CB	3:AAA:403:GOL:H12	1.99	0.86
1:CCC:280:PHE:O	1:CCC:282:GLU:HG3	1.76	0.86
2:DDD:407:EDO:H22	5:DDD:592:HOH:O	1.75	0.85
1:AAA:287:GLN:O	1:AAA:291:GLU:HG3	1.83	0.79
1:DDD:46:GLU:HB2	3:DDD:401:GOL:C1	2.12	0.78
1:AAA:296:THR:HB	3:AAA:403:GOL:C1	1.99	0.78
1:DDD:128[B]:ARG:NH1	1:DDD:261:GLU:OE1	2.21	0.74
1:BBB:164:ARG:HE	2:BBB:403:EDO:H22	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:53[B]:ILE:HG12	1:AAA:57:ASN:HB2	1.73	0.70
1:AAA:279:VAL:O	1:AAA:293:TYR:OH	2.03	0.69
1:CCC:296:THR:HB	3:CCC:504:GOL:H12	1.73	0.68
1:AAA:53[A]:ILE:HG22	1:DDD:92:SER:OG	1.96	0.65
1:DDD:56:GLN:HB2	1:DDD:88[B]:ILE:CD1	2.27	0.65
1:DDD:88[B]:ILE:HD12	5:DDD:546:HOH:O	1.98	0.63
1:CCC:51:MET:HE1	1:CCC:61:VAL:HG11	1.81	0.62
1:BBB:121[B]:ILE:HD12	1:BBB:250:SER:HB2	1.81	0.62
1:AAA:231[A]:GLU:HG2	5:AAA:559:HOH:O	2.01	0.61
1:BBB:287:GLN:O	1:BBB:291:GLU:HG2	2.01	0.60
1:CCC:56:GLN:HB2	1:CCC:88[A]:ILE:HD12	1.83	0.60
1:BBB:53:ILE:HG13	1:CCC:88[B]:ILE:CD1	2.35	0.57
1:BBB:46:GLU:HB2	3:BBB:405:GOL:H12	1.88	0.55
1:BBB:171:PHE:HB3	1:BBB:175[B]:ILE:HD12	1.89	0.55
1:BBB:164:ARG:HH21	1:BBB:164:ARG:HG2	1.72	0.53
1:CCC:108:GLY:H	2:CCC:503:EDO:H21	1.73	0.53
1:CCC:171:PHE:HA	2:CCC:502:EDO:H21	1.89	0.53
1:DDD:56:GLN:HB2	1:DDD:88[B]:ILE:HD13	1.89	0.53
1:BBB:279:VAL:HG11	5:DDD:581:HOH:O	2.07	0.53
1:CCC:297:ALA:H	3:CCC:504:GOL:H31	1.73	0.53
1:AAA:10:TYR:CZ	1:AAA:14:LEU:HD11	2.44	0.52
1:BBB:53:ILE:HG13	1:CCC:88[B]:ILE:HD12	1.90	0.52
1:BBB:10:TYR:CZ	1:BBB:14:LEU:HD11	2.45	0.52
1:CCC:10:TYR:CZ	1:CCC:14:LEU:HD11	2.45	0.52
1:BBB:164:ARG:NH2	1:BBB:164:ARG:HG2	2.25	0.51
1:DDD:10:TYR:CZ	1:DDD:14:LEU:HD11	2.46	0.51
1:BBB:287:GLN:O	1:BBB:291:GLU:CG	2.59	0.50
1:BBB:154[A]:ILE:HD11	1:BBB:179:PRO:HG3	1.93	0.49
1:BBB:47[A]:ARG:HD3	3:BBB:405:GOL:O2	2.12	0.49
1:AAA:298[A]:ARG:NH2	3:AAA:403:GOL:H11	2.27	0.49
1:AAA:95:TYR:HE1	1:CCC:279:VAL:HG11	1.77	0.49
1:AAA:48:PHE:CE2	1:AAA:50:ASN:HB2	2.48	0.48
1:AAA:7[A]:ARG:NH1	5:AAA:501:HOH:O	2.46	0.48
1:DDD:56:GLN:HB2	1:DDD:88[B]:ILE:HD12	1.95	0.48
1:BBB:70:LYS:CE	5:BBB:579:HOH:O	2.61	0.48
1:DDD:282:GLU:C	1:DDD:284:GLY:H	2.16	0.48
1:DDD:239[B]:LEU:HD23	1:DDD:240:THR:HG23	1.96	0.47
1:BBB:48:PHE:CE2	1:BBB:50:ASN:HB2	2.50	0.47
1:AAA:55:GLU:HG3	1:AAA:80:PHE:CD2	2.51	0.46
1:DDD:312:ARG:HD3	5:DDD:563:HOH:O	2.16	0.46
1:AAA:24:ILE:O	1:AAA:47[B]:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:48:PHE:CE2	1:DDD:50:ASN:HB2	2.51	0.46
1:BBB:265:GLU:OE2	1:DDD:273[A]:LYS:HE2	2.17	0.45
1:AAA:108:GLY:H	2:AAA:404:EDO:H11	1.81	0.45
1:BBB:55:GLU:HG3	1:BBB:80:PHE:CD2	2.52	0.45
1:DDD:51:MET:HE3	1:DDD:58:LEU:HD12	1.99	0.45
1:CCC:55:GLU:HG3	1:CCC:80:PHE:CD2	2.52	0.45
1:CCC:282:GLU:OE2	1:CCC:292:LYS:HD2	2.18	0.44
1:CCC:154[B]:ILE:HD11	1:CCC:179:PRO:CG	2.48	0.44
1:CCC:48:PHE:CE2	1:CCC:50:ASN:HB2	2.52	0.44
1:CCC:154[B]:ILE:HD11	1:CCC:179:PRO:HG3	2.00	0.43
1:DDD:88[A]:ILE:HG13	1:DDD:92:SER:HB2	2.00	0.43
1:DDD:154[B]:ILE:HD11	1:DDD:179:PRO:HG3	2.00	0.43
1:DDD:47[A]:ARG:HD3	3:DDD:401:GOL:H2	2.00	0.43
1:BBB:24:ILE:O	1:BBB:47[B]:ARG:HD2	2.19	0.42
1:CCC:296:THR:HA	3:CCC:504:GOL:H31	2.00	0.42
1:DDD:154[B]:ILE:HD11	1:DDD:179:PRO:CG	2.49	0.42
1:AAA:79[B]:VAL:HG21	1:AAA:118[B]:HIS:HA	2.01	0.42
1:BBB:88:ILE:HG13	1:BBB:92:SER:HB2	2.02	0.42
1:CCC:196:LEU:HG	1:CCC:255:LEU:HD22	2.02	0.41
1:AAA:154[B]:ILE:HD11	1:AAA:179:PRO:CG	2.50	0.41
1:BBB:202:LYS:HE3	1:BBB:290:LEU:HD21	2.01	0.41
1:DDD:164:ARG:NH1	5:DDD:502:HOH:O	2.53	0.41
1:AAA:121:ILE:HD13	1:AAA:250:SER:HB2	2.03	0.41
1:AAA:69:GLY:N	5:AAA:502:HOH:O	2.52	0.41
1:AAA:154[B]:ILE:HD11	1:AAA:179:PRO:HG3	2.03	0.41
1:BBB:154[A]:ILE:HD11	1:BBB:179:PRO:CG	2.51	0.40
1:DDD:47[A]:ARG:HD3	3:DDD:401:GOL:C2	2.52	0.40
1:DDD:51:MET:CE	1:DDD:58:LEU:HD12	2.52	0.40

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	AAA	320/341 (94%)	309 (97%)	10 (3%)	1 (0%)	41	31
1	BBB	310/341 (91%)	301 (97%)	9 (3%)	0	100	100
1	CCC	316/341 (93%)	308 (98%)	8 (2%)	0	100	100
1	DDD	329/341 (96%)	313 (95%)	14 (4%)	2 (1%)	25	15
All	All	1275/1364 (94%)	1231 (96%)	41 (3%)	3 (0%)	41	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	279	VAL
1	DDD	283	SER
1	DDD	112	GLY

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	AAA	256/260 (98%)	246 (96%)	10 (4%)	32	23
1	BBB	246/260 (95%)	238 (97%)	8 (3%)	38	29
1	CCC	251/260 (96%)	242 (96%)	9 (4%)	35	26
1	DDD	258/260 (99%)	245 (95%)	13 (5%)	24	15
All	All	1011/1040 (97%)	971 (96%)	40 (4%)	34	22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	34[A]	SER
1	AAA	34[B]	SER
1	AAA	51[A]	MET
1	AAA	51[B]	MET
1	AAA	175	ILE
1	AAA	176	ARG
1	AAA	196	LEU
1	AAA	280	PHE

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Mol	Chain	Res	Type
1	AAA	285	THR
1	AAA	312	ARG
1	BBB	33	LYS
1	BBB	51[A]	MET
1	BBB	51[B]	MET
1	BBB	161	ARG
1	BBB	164	ARG
1	BBB	175[A]	ILE
1	BBB	175[B]	ILE
1	BBB	196	LEU
1	CCC	33	LYS
1	CCC	51	MET
1	CCC	145	ARG
1	CCC	161	ARG
1	CCC	175[A]	ILE
1	CCC	175[B]	ILE
1	CCC	196	LEU
1	CCC	208	LYS
1	CCC	289	LEU
1	DDD	33	LYS
1	DDD	111	VAL
1	DDD	113	GLU
1	DDD	114	ASP
1	DDD	117	SER
1	DDD	119[A]	GLN
1	DDD	119[B]	GLN
1	DDD	161	ARG
1	DDD	164	ARG
1	DDD	175	ILE
1	DDD	196	LEU
1	DDD	292	LYS
1	DDD	306	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	BBB	402	-	3,3,3	0.10	0	2,2,2	0.12	0
2	EDO	DDD	403	-	3,3,3	0.17	0	2,2,2	0.29	0
2	EDO	AAA	402	-	3,3,3	0.17	0	2,2,2	0.72	0
3	GOL	DDD	406	-	5,5,5	0.12	0	5,5,5	0.49	0
2	EDO	AAA	404	-	3,3,3	0.24	0	2,2,2	0.17	0
2	EDO	DDD	407	-	3,3,3	0.12	0	2,2,2	0.47	0
3	GOL	AAA	403	-	5,5,5	0.07	0	5,5,5	0.32	0
2	EDO	CCC	502	-	3,3,3	0.16	0	2,2,2	0.20	0
2	EDO	BBB	403	-	3,3,3	0.16	0	2,2,2	0.60	0
2	EDO	CCC	503	-	3,3,3	0.19	0	2,2,2	0.44	0
3	GOL	BBB	405	-	5,5,5	0.10	0	5,5,5	0.33	0
2	EDO	DDD	402	-	3,3,3	0.04	0	2,2,2	0.11	0
3	GOL	BBB	401	-	5,5,5	0.12	0	5,5,5	0.34	0
2	EDO	CCC	501	-	3,3,3	0.19	0	2,2,2	0.51	0
2	EDO	DDD	405	-	3,3,3	0.10	0	2,2,2	0.22	0
2	EDO	DDD	404	-	3,3,3	0.24	0	2,2,2	0.67	0
3	GOL	DDD	401	-	5,5,5	0.13	0	5,5,5	0.39	0
4	PEG	BBB	406	-	6,6,6	0.38	0	5,5,5	0.22	0
2	EDO	AAA	405	-	3,3,3	0.17	0	2,2,2	0.51	0
3	GOL	CCC	504	-	5,5,5	0.13	0	5,5,5	0.63	0
2	EDO	AAA	401	-	3,3,3	0.08	0	2,2,2	0.40	0
2	EDO	BBB	404	-	3,3,3	0.22	0	2,2,2	0.50	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
2	EDO	BBB	402	-	-	1/1/1/1	-
2	EDO	DDD	403	-	-	1/1/1/1	-
2	EDO	AAA	402	-	-	0/1/1/1	-
3	GOL	DDD	406	-	-	4/4/4/4	-
2	EDO	AAA	404	-	-	1/1/1/1	-
2	EDO	DDD	407	-	-	0/1/1/1	-
3	GOL	AAA	403	-	-	2/4/4/4	-
2	EDO	CCC	502	-	-	0/1/1/1	-
2	EDO	BBB	403	-	-	1/1/1/1	-
2	EDO	CCC	503	-	-	1/1/1/1	-
3	GOL	BBB	405	-	-	2/4/4/4	-
2	EDO	DDD	402	-	-	1/1/1/1	-
3	GOL	BBB	401	-	-	2/4/4/4	-
2	EDO	CCC	501	-	-	0/1/1/1	-
2	EDO	DDD	405	-	-	1/1/1/1	-
2	EDO	DDD	404	-	-	1/1/1/1	-
3	GOL	DDD	401	-	-	2/4/4/4	-
4	PEG	BBB	406	-	-	3/4/4/4	-
2	EDO	AAA	405	-	-	1/1/1/1	-
3	GOL	CCC	504	-	-	2/4/4/4	-
2	EDO	AAA	401	-	-	1/1/1/1	-
2	EDO	BBB	404	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DDD	406	GOL	O1-C1-C2-O2
3	DDD	406	GOL	O1-C1-C2-C3
3	BBB	405	GOL	O1-C1-C2-O2
3	BBB	405	GOL	O1-C1-C2-C3
3	BBB	401	GOL	C1-C2-C3-O3
3	CCC	504	GOL	O1-C1-C2-C3
4	BBB	406	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	DDD	406	GOL	O2-C2-C3-O3
3	BBB	401	GOL	O2-C2-C3-O3
3	DDD	406	GOL	C1-C2-C3-O3
3	AAA	403	GOL	C1-C2-C3-O3
3	DDD	401	GOL	O1-C1-C2-C3
3	CCC	504	GOL	O1-C1-C2-O2
2	BBB	402	EDO	O1-C1-C2-O2
2	DDD	403	EDO	O1-C1-C2-O2
2	BBB	403	EDO	O1-C1-C2-O2
2	DDD	404	EDO	O1-C1-C2-O2
2	AAA	405	EDO	O1-C1-C2-O2
2	AAA	401	EDO	O1-C1-C2-O2
4	BBB	406	PEG	C1-C2-O2-C3
2	DDD	405	EDO	O1-C1-C2-O2
4	BBB	406	PEG	C4-C3-O2-C2
2	DDD	402	EDO	O1-C1-C2-O2
2	CCC	503	EDO	O1-C1-C2-O2
3	AAA	403	GOL	O2-C2-C3-O3
2	AAA	404	EDO	O1-C1-C2-O2
3	DDD	401	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	404	EDO	1	0
2	DDD	407	EDO	1	0
3	AAA	403	GOL	4	0
2	CCC	502	EDO	1	0
2	BBB	403	EDO	1	0
2	CCC	503	EDO	1	0
3	BBB	405	GOL	2	0
3	DDD	401	GOL	4	0
3	CCC	504	GOL	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	AAA	303/341 (88%)	0.35	24 (7%)	12 14	37, 51, 110, 178	0
1	BBB	299/341 (87%)	0.45	23 (7%)	13 15	40, 52, 101, 175	0
1	CCC	300/341 (87%)	0.45	28 (9%)	8 10	39, 54, 99, 179	0
1	DDD	311/341 (91%)	0.41	16 (5%)	28 31	38, 50, 107, 165	0
All	All	1213/1364 (88%)	0.41	91 (7%)	14 15	37, 52, 108, 179	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	283	SER	8.7
1	AAA	280	PHE	8.3
1	CCC	280	PHE	8.0
1	DDD	112	GLY	7.4
1	DDD	114	ASP	7.3
1	AAA	286	PRO	6.5
1	AAA	290	LEU	6.2
1	AAA	287	GLN	6.2
1	AAA	285	THR	6.1
1	CCC	289	LEU	5.7
1	DDD	2	GLY	5.3
1	DDD	111	VAL	5.1
1	BBB	287	GLN	5.1
1	BBB	279	VAL	5.1
1	AAA	116	ALA	4.9
1	AAA	288	ALA	4.8
1	BBB	2	GLY	4.7
1	CCC	288	ALA	4.7
1	CCC	2	GLY	4.7
1	CCC	37	THR	4.5
1	CCC	290	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	294	GLY	4.4
1	BBB	33	LYS	4.4
1	CCC	279	VAL	4.2
1	AAA	289	LEU	4.1
1	AAA	282	GLU	4.1
1	CCC	278	ASP	4.1
1	BBB	289	LEU	4.0
1	DDD	37	THR	3.8
1	DDD	110	THR	3.8
1	CCC	212	ALA	3.7
1	BBB	288	ALA	3.7
1	AAA	291	GLU	3.7
1	DDD	113	GLU	3.6
1	CCC	115	GLY	3.5
1	BBB	31	LEU	3.5
1	CCC	215	ILE	3.4
1	CCC	211[A]	GLU	3.4
1	DDD	33	LYS	3.4
1	CCC	35	THR	3.3
1	CCC	33	LYS	3.3
1	CCC	164	ARG	3.2
1	AAA	115	GLY	3.1
1	CCC	282	GLU	3.1
1	AAA	212	ALA	3.1
1	DDD	211[A]	GLU	3.1
1	BBB	286	PRO	3.1
1	BBB	37	THR	3.1
1	DDD	31	LEU	3.1
1	DDD	34[A]	SER	3.0
1	CCC	291	GLU	3.0
1	AAA	278	ASP	3.0
1	BBB	4	ILE	2.9
1	AAA	312	ARG	2.8
1	AAA	281	GLY	2.8
1	CCC	281	GLY	2.8
1	BBB	116	ALA	2.7
1	CCC	39	ASP	2.6
1	CCC	32[A]	SER	2.6
1	AAA	4	ILE	2.6
1	AAA	3	GLY	2.6
1	BBB	293	TYR	2.6
1	CCC	292	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	129	VAL	2.6
1	DDD	251	VAL	2.6
1	BBB	3	GLY	2.5
1	CCC	312	ARG	2.5
1	CCC	213[A]	GLU	2.5
1	AAA	211[A]	GLU	2.5
1	CCC	31	LEU	2.5
1	DDD	252	ILE	2.5
1	AAA	31	LEU	2.4
1	BBB	34[A]	SER	2.4
1	DDD	42	LYS	2.4
1	AAA	118[A]	HIS	2.4
1	CCC	4	ILE	2.4
1	BBB	290	LEU	2.4
1	AAA	293	TYR	2.3
1	CCC	107	ALA	2.3
1	AAA	279	VAL	2.3
1	CCC	3	GLY	2.3
1	BBB	255	LEU	2.3
1	DDD	214	GLY	2.3
1	BBB	42	LYS	2.3
1	BBB	115	GLY	2.2
1	BBB	118[A]	HIS	2.2
1	AAA	117	SER	2.2
1	BBB	8	GLU	2.1
1	BBB	278	ASP	2.1
1	CCC	293	TYR	2.1
1	DDD	3	GLY	2.1

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 monosaccharides 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
2	EDO	AAA	404	4/4	0.61	0.18	90,93,101,102	0
3	GOL	AAA	403	6/6	0.66	0.18	98,100,103,105	0
4	PEG	BBB	406	7/7	0.66	0.18	77,85,99,108	0
3	GOL	BBB	401	6/6	0.75	0.17	79,106,109,109	0
2	EDO	DDD	402	4/4	0.75	0.22	100,112,122,122	0
2	EDO	AAA	405	4/4	0.79	0.13	89,96,105,114	0
3	GOL	DDD	406	6/6	0.82	0.27	58,76,94,98	0
2	EDO	CCC	502	4/4	0.82	0.22	76,78,85,89	0
2	EDO	BBB	403	4/4	0.83	0.25	93,97,98,103	0
3	GOL	BBB	405	6/6	0.83	0.24	64,75,82,83	6
3	GOL	DDD	401	6/6	0.84	0.35	60,84,89,93	0
2	EDO	CCC	503	4/4	0.84	0.26	85,98,102,104	0
2	EDO	DDD	404	4/4	0.84	0.24	75,79,81,92	0
2	EDO	DDD	405	4/4	0.85	0.13	94,95,100,103	0
2	EDO	AAA	402	4/4	0.87	0.13	77,81,81,85	0
2	EDO	BBB	404	4/4	0.88	0.18	79,84,87,94	0
2	EDO	BBB	402	4/4	0.90	0.08	80,97,104,108	0
3	GOL	CCC	504	6/6	0.91	0.12	80,90,97,121	0
2	EDO	DDD	403	4/4	0.91	0.16	92,95,95,99	0
2	EDO	AAA	401	4/4	0.93	0.11	65,82,92,93	0
2	EDO	CCC	501	4/4	0.94	0.19	74,88,89,97	0
2	EDO	DDD	407	4/4	0.96	0.14	70,86,93,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.