



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:05 AM UTC

PDB ID : 2ASH / pdb_00002ash
Title : Crystal structure of Queuine tRNA-ribosyltransferase (EC 2.4.2.29) (tRNA-guanine (tm1561) from THERMOTOGA MARITIMA at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2005-08-23
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 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

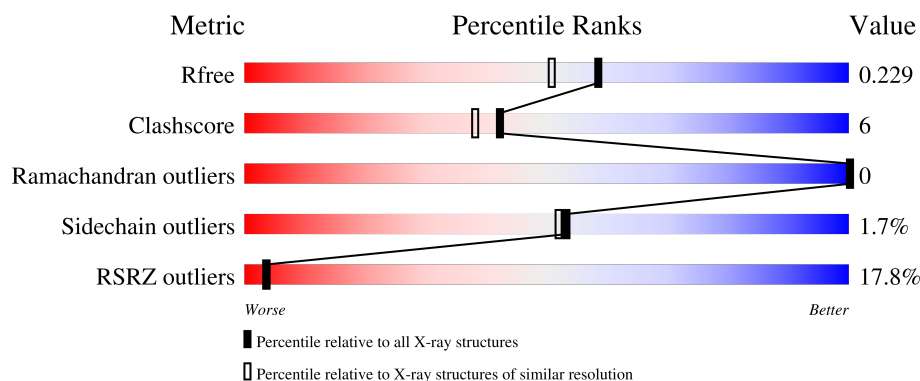
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	381	20% 82% 12% • 5%
1	B	381	7% 86% 8% • 6%
1	C	381	30% 79% 14% • 5%
1	D	381	11% 84% 10% 5%

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	EDO	B	401	-	-	X	-
4	EDO	C	405	-	-	X	-
4	EDO	D	402[A]	-	-	X	-
4	EDO	D	402[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11856 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 Queuine tRNA-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	6	0
			2794	1805	474	499	16			
1	B	360	Total	C	N	O	S	0	6	0
			2804	1811	470	507	16			
1	C	361	Total	C	N	O	S	0	5	0
			2756	1780	464	496	16			
1	D	361	Total	C	N	O	S	0	2	0
			2794	1804	476	498	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9X1P7
A	-10	GLY	-	expression tag	UNP Q9X1P7
A	-9	SER	-	expression tag	UNP Q9X1P7
A	-8	ASP	-	expression tag	UNP Q9X1P7
A	-7	LYS	-	expression tag	UNP Q9X1P7
A	-6	ILE	-	expression tag	UNP Q9X1P7
A	-5	HIS	-	expression tag	UNP Q9X1P7
A	-4	HIS	-	expression tag	UNP Q9X1P7
A	-3	HIS	-	expression tag	UNP Q9X1P7
A	-2	HIS	-	expression tag	UNP Q9X1P7
A	-1	HIS	-	expression tag	UNP Q9X1P7
A	0	HIS	-	expression tag	UNP Q9X1P7
B	-11	MET	-	expression tag	UNP Q9X1P7
B	-10	GLY	-	expression tag	UNP Q9X1P7
B	-9	SER	-	expression tag	UNP Q9X1P7
B	-8	ASP	-	expression tag	UNP Q9X1P7
B	-7	LYS	-	expression tag	UNP Q9X1P7
B	-6	ILE	-	expression tag	UNP Q9X1P7
B	-5	HIS	-	expression tag	UNP Q9X1P7
B	-4	HIS	-	expression tag	UNP Q9X1P7
B	-3	HIS	-	expression tag	UNP Q9X1P7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9X1P7
B	-1	HIS	-	expression tag	UNP Q9X1P7
B	0	HIS	-	expression tag	UNP Q9X1P7
C	-11	MET	-	expression tag	UNP Q9X1P7
C	-10	GLY	-	expression tag	UNP Q9X1P7
C	-9	SER	-	expression tag	UNP Q9X1P7
C	-8	ASP	-	expression tag	UNP Q9X1P7
C	-7	LYS	-	expression tag	UNP Q9X1P7
C	-6	ILE	-	expression tag	UNP Q9X1P7
C	-5	HIS	-	expression tag	UNP Q9X1P7
C	-4	HIS	-	expression tag	UNP Q9X1P7
C	-3	HIS	-	expression tag	UNP Q9X1P7
C	-2	HIS	-	expression tag	UNP Q9X1P7
C	-1	HIS	-	expression tag	UNP Q9X1P7
C	0	HIS	-	expression tag	UNP Q9X1P7
D	-11	MET	-	expression tag	UNP Q9X1P7
D	-10	GLY	-	expression tag	UNP Q9X1P7
D	-9	SER	-	expression tag	UNP Q9X1P7
D	-8	ASP	-	expression tag	UNP Q9X1P7
D	-7	LYS	-	expression tag	UNP Q9X1P7
D	-6	ILE	-	expression tag	UNP Q9X1P7
D	-5	HIS	-	expression tag	UNP Q9X1P7
D	-4	HIS	-	expression tag	UNP Q9X1P7
D	-3	HIS	-	expression tag	UNP Q9X1P7
D	-2	HIS	-	expression tag	UNP Q9X1P7
D	-1	HIS	-	expression tag	UNP Q9X1P7
D	0	HIS	-	expression tag	UNP Q9X1P7

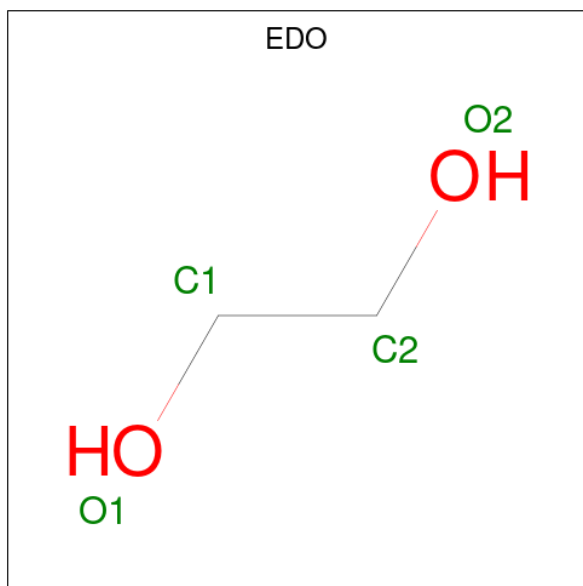
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 6 3 3	0	1
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 6 3 3	0	1

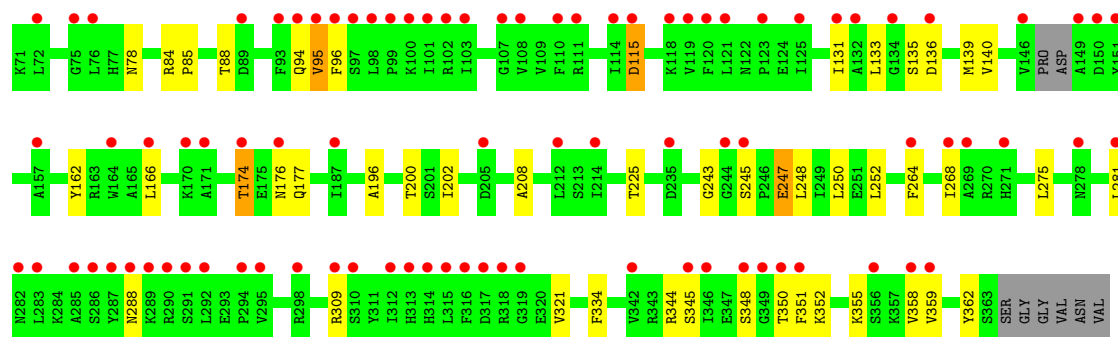
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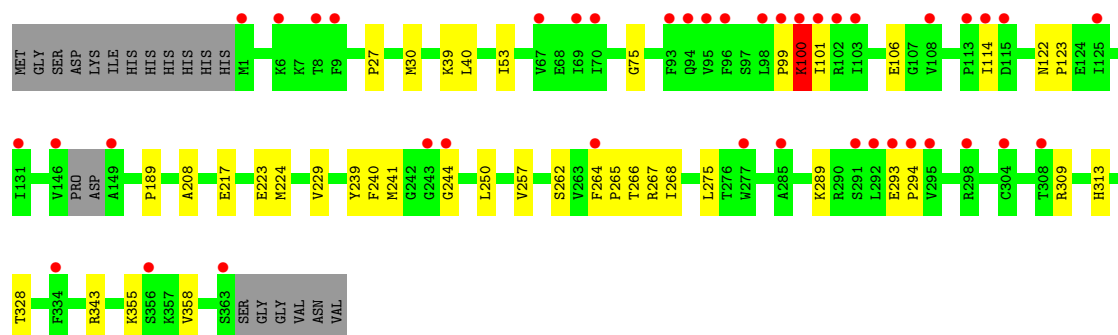
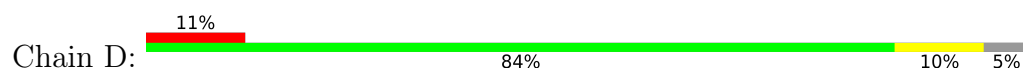
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	210	Total	O	0	0
			210	210		
5	C	126	Total	O	0	0
			126	126		
5	D	163	Total	O	0	0
			163	163		



● Molecule 1: Queuine tRNA-ribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 99.42Å 124.16Å 90.00° 123.80° 90.00°	Depositor
Resolution (Å)	51.70 – 1.90 51.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (51.70-1.90) 97.6 (51.70-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.193 , 0.229 0.196 , 0.229	Depositor DCC
R_{free} test set	6626 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11856	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: CL, ZN, 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	A	1.03	0/2877	1.05	4/3889 (0.1%)
1	B	1.04	1/2887 (0.0%)	0.97	1/3901 (0.0%)
1	C	1.01	4/2835 (0.1%)	0.99	3/3838 (0.1%)
1	D	1.18	1/2861 (0.0%)	1.08	6/3866 (0.2%)
All	All	1.07	6/11460 (0.1%)	1.02	14/15494 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	100	LYS	C-O	30.35	1.68	1.23
1	B	264	PHE	C-O	-6.73	1.18	1.24
1	C	352	LYS	C-O	6.37	1.32	1.24
1	C	334	PHE	C-O	-5.34	1.18	1.24
1	C	78	ASN	C-O	-5.31	1.17	1.24
1	C	140	VAL	CA-CB	5.18	1.59	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	LYS	O-C-N	-18.23	100.17	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	LYS	CA-C-N	13.94	137.19	122.27
1	D	100	LYS	C-N-CA	13.94	137.19	122.27
1	C	115	ASP	CA-CB-CG	8.24	120.84	112.60
1	A	59	PHE	N-CA-C	-8.13	102.35	111.14
1	A	75	GLY	N-CA-C	6.98	118.58	111.95
1	D	99	PRO	O-C-N	6.70	131.30	123.06
1	A	85	PRO	N-CA-C	5.83	120.47	111.21
1	D	100	LYS	N-CA-C	5.53	117.93	111.02
1	B	100	LYS	N-CA-C	5.50	117.90	111.02
1	A	202	ILE	N-CA-C	-5.50	106.33	111.45
1	D	75	GLY	N-CA-C	5.30	117.44	112.08
1	C	344	ARG	CA-C-N	5.06	127.06	120.28
1	C	344	ARG	C-N-CA	5.06	127.06	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	362	TYR	Peptide
1	D	100	LYS	Mainchain

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	2794	0	2753	37	0
1	B	2804	0	2763	29	0
1	C	2756	0	2683	42	0
1	D	2794	0	2760	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	5	6	0
4	C	16	0	23	4	0
4	D	10	0	18	11	0
5	A	156	0	0	3	0
5	B	210	0	0	4	0
5	C	126	0	0	2	0
5	D	163	0	0	5	0
All	All	11856	0	11029	141	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 6.

All (141) 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:D:100:LYS:C	1:D:100:LYS:O	1.68	1.34
1:C:247[A]:GLU:OE1	1:C:362:TYR:HB3	1.65	0.97
1:B:131:ILE:HG23	1:B:174[B]:THR:CG2	2.02	0.90
1:A:131:ILE:HG23	1:A:174[B]:THR:HG21	1.55	0.86
1:A:131:ILE:HG23	1:A:174[B]:THR:CG2	2.06	0.86
1:C:65:PRO:HB3	4:D:402[A]:EDO:O2	1.79	0.82
1:B:174[A]:THR:HG21	1:B:177:GLN:OE1	1.80	0.82
1:B:320:GLU:OE1	4:B:401:EDO:H11	1.80	0.81
1:A:196:ALA:O	1:A:200:THR:HB	1.82	0.80
1:C:348[A]:SER:OG	1:C:350:THR:HG22	1.84	0.78
1:D:250:LEU:HD23	1:D:355:LYS:HA	1.70	0.72
1:B:131:ILE:HG12	1:B:174[B]:THR:HG21	1.71	0.72
1:C:250:LEU:HD23	1:C:355:LYS:HA	1.73	0.70
1:C:281:LEU:HD21	1:C:309:ARG:HD3	1.75	0.69
1:B:189:PRO:HG3	1:B:224:MET:HE1	1.75	0.68
1:B:131:ILE:HG23	1:B:174[B]:THR:HG21	1.77	0.67
1:B:223:GLU:HG2	1:B:224:MET:HE2	1.76	0.67
1:C:95:VAL:HG12	1:C:96:PHE:CD2	2.31	0.65
1:B:131:ILE:HG23	1:B:174[B]:THR:HG22	1.76	0.64
1:B:131:ILE:HG12	1:B:174[B]:THR:CG2	2.28	0.64
1:B:131:ILE:CG2	1:B:174[B]:THR:CG2	2.75	0.63
1:C:345[A]:SER:HB2	1:C:351:PHE:HA	1.80	0.63
1:A:39:LYS:HG2	4:B:401:EDO:H22	1.82	0.62
1:D:294:PRO:O	1:D:309:ARG:HD2	2.00	0.61
1:A:131:ILE:CG2	1:A:174[B]:THR:CG2	2.79	0.61
1:B:243:GLY:O	1:B:248:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LYS:O	1:D:101:ILE:N	2.32	0.60
1:D:223:GLU:HG2	1:D:224:MET:HE2	1.84	0.60
1:A:59:PHE:CE1	1:A:95:VAL:HG22	2.37	0.58
1:A:96:PHE:CZ	1:A:108[A]:VAL:HG21	2.39	0.58
1:D:267:ARG:CD	5:D:466:HOH:O	2.51	0.58
1:B:362:TYR:O	1:B:363:SER:C	2.47	0.58
1:B:149:ALA:HB1	1:B:153:GLU:CD	2.30	0.57
1:D:313:HIS:HD2	4:D:402[B]:EDO:H12	1.69	0.57
1:D:266:THR:HG22	1:D:328:THR:HG23	1.86	0.57
1:C:131:ILE:HG23	1:C:174:THR:CG2	2.35	0.56
1:C:245:SER:HB2	1:C:247[A]:GLU:OE2	2.06	0.56
1:C:247[A]:GLU:HG2	1:C:248:LEU:H	1.71	0.56
4:C:405:EDO:H21	1:D:40:LEU:HD23	1.88	0.55
1:A:30:MET:HG2	1:A:53:ILE:HG23	1.87	0.55
1:A:27:PRO:HD2	1:A:343:ARG:HG2	1.87	0.55
1:C:174:THR:HG21	1:C:177:GLN:OE1	2.07	0.55
1:D:313:HIS:HD2	4:D:402[A]:EDO:H12	1.71	0.54
1:C:59:PHE:CE1	1:C:95:VAL:HG23	2.42	0.54
1:A:52:GLU:O	1:A:85:PRO:HD2	2.07	0.54
1:D:293:GLU:HB2	1:D:309:ARG:HD3	1.88	0.54
1:B:174[A]:THR:HG22	1:B:175:GLU:H	1.73	0.53
1:C:250:LEU:HD22	1:C:358:VAL:HB	1.90	0.53
1:D:106:GLU:CG	5:D:480:HOH:O	2.57	0.52
1:D:240:PHE:HB2	1:D:257:VAL:HG11	1.92	0.52
1:D:241:MET:HE3	5:D:525:HOH:O	2.10	0.52
1:D:289:LYS:HG2	4:D:402[B]:EDO:H11	1.91	0.52
1:B:60:HIS:HD2	5:B:438:HOH:O	1.93	0.52
1:B:320:GLU:OE1	4:B:401:EDO:C1	2.57	0.52
1:C:321:VAL:HB	4:C:405:EDO:H22	1.90	0.51
1:A:244:GLY:HA3	1:A:262:SER:HB2	1.92	0.51
1:B:264:PHE:HD2	5:B:597:HOH:O	1.92	0.51
1:C:65:PRO:HB3	4:D:402[A]:EDO:HO2	1.72	0.51
1:C:70:ILE:HG21	1:C:133:LEU:HD23	1.93	0.51
1:D:289:LYS:HG2	4:D:402[A]:EDO:H11	1.93	0.51
1:C:288:ASN:OD1	1:C:309:ARG:HD2	2.10	0.50
1:D:313:HIS:CD2	4:D:402[B]:EDO:H12	2.47	0.50
1:A:362:TYR:O	1:A:363:SER:C	2.54	0.50
1:A:150:ASP:CG	1:A:153:GLU:OE2	2.55	0.50
1:C:162:TYR:CZ	1:C:166:LEU:HD11	2.47	0.50
1:C:59:PHE:HE1	1:C:95:VAL:HG23	1.76	0.49
1:B:268:ILE:HD11	1:B:275:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASP:HB3	5:A:455:HOH:O	2.11	0.48
1:D:313:HIS:CD2	4:D:402[A]:EDO:H12	2.48	0.48
1:C:247[A]:GLU:HG2	1:C:248:LEU:N	2.28	0.48
1:A:131:ILE:HG12	1:A:174[B]:THR:HG21	1.94	0.48
1:C:243:GLY:O	1:C:248:LEU:HD23	2.13	0.48
1:C:94:GLN:HG2	5:C:452:HOH:O	2.13	0.48
1:C:162:TYR:CE1	1:C:202:ILE:HD11	2.48	0.48
1:D:264:PHE:HD2	5:D:509:HOH:O	1.95	0.48
1:A:39:LYS:HB3	4:B:401:EDO:H21	1.95	0.48
1:A:266:THR:HG22	1:A:328:THR:HG23	1.96	0.47
1:B:103:ILE:HG23	1:B:108[A]:VAL:HG22	1.96	0.47
1:A:297:GLU:CG	5:A:543:HOH:O	2.63	0.47
1:B:34:THR:O	5:B:595:HOH:O	2.20	0.47
1:C:245:SER:CB	1:C:247[A]:GLU:OE2	2.63	0.47
1:B:103:ILE:CG1	1:B:108[A]:VAL:HG22	2.45	0.47
1:D:264:PHE:O	1:D:268:ILE:HG12	2.15	0.47
1:A:8[A]:THR:HG22	5:A:544:HOH:O	2.15	0.46
1:D:217:GLU:CG	5:D:496:HOH:O	2.63	0.45
1:B:131:ILE:HG12	1:B:174[A]:THR:OG1	2.16	0.45
1:C:264:PHE:O	1:C:268:ILE:HG23	2.17	0.45
1:A:9:PHE:HD2	1:A:351:PHE:HB3	1.82	0.45
1:C:264:PHE:HD2	5:C:467:HOH:O	1.98	0.44
1:C:84:ARG:HB3	1:C:85:PRO:CD	2.47	0.44
1:A:39:LYS:CG	4:B:401:EDO:H22	2.47	0.44
1:A:96:PHE:CE1	1:A:108[A]:VAL:HG21	2.52	0.44
1:C:88:THR:HG23	1:C:135:SER:HB3	2.00	0.44
1:D:250:LEU:HD22	1:D:358:VAL:HB	1.99	0.44
1:A:250:LEU:HD22	1:A:355:LYS:HA	1.99	0.44
1:B:26:THR:HA	1:B:27:PRO:C	2.43	0.44
1:B:305:LYS:CD	5:B:485:HOH:O	2.66	0.44
1:C:65:PRO:CB	4:D:402[A]:EDO:O2	2.59	0.44
1:C:139:MET:HE1	1:C:208:ALA:HB2	2.00	0.44
1:C:30:MET:HG2	1:C:53:ILE:HG23	1.99	0.43
1:A:4:GLU:O	1:A:15:GLY:HA2	2.18	0.43
1:A:57[B]:ASN:OD1	1:A:58:THR:N	2.51	0.43
1:C:26:THR:HA	1:C:27:PRO:C	2.42	0.43
1:C:131:ILE:HG23	1:C:174:THR:HG21	1.99	0.43
1:A:9:PHE:CD2	1:A:351:PHE:HB3	2.53	0.43
1:C:225:THR:HG21	1:C:252:LEU:HD22	2.01	0.43
1:A:131:ILE:CG2	1:A:174[B]:THR:HG21	2.35	0.43
1:A:58:THR:HG22	1:A:133:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ILE:HD11	1:C:275:LEU:HD21	2.01	0.42
1:D:27:PRO:HD2	1:D:343:ARG:HG2	2.01	0.42
1:B:266:THR:HG22	1:B:328:THR:HG23	2.02	0.42
1:D:244:GLY:HA3	1:D:262:SER:HB2	2.01	0.42
1:D:289:LYS:CG	4:D:402[B]:EDO:H11	2.48	0.42
1:C:85:PRO:HA	1:C:136:ASP:OD1	2.19	0.42
1:A:250:LEU:CD2	1:A:355:LYS:HA	2.50	0.42
1:D:189:PRO:HG3	1:D:224:MET:HE1	2.00	0.42
1:A:7:LYS:HD3	1:A:347:GLU:HA	2.01	0.42
1:C:20:HIS:CG	1:C:176:ASN:HB3	2.55	0.42
1:C:196:ALA:O	1:C:200:THR:HG23	2.19	0.42
1:C:345[B]:SER:HB3	1:C:351:PHE:HA	2.00	0.42
1:A:290[B]:ARG:HH12	1:B:68[B]:GLU:CD	2.28	0.42
4:C:405:EDO:H12	1:D:39:LYS:HD3	2.02	0.42
1:B:85:PRO:HA	1:B:136:ASP:OD1	2.20	0.41
1:D:30:MET:HG2	1:D:53:ILE:HG23	2.02	0.41
1:A:27:PRO:HA	1:A:258:ASP:O	2.20	0.41
1:D:264:PHE:N	1:D:265:PRO:HD2	2.34	0.41
4:C:405:EDO:C2	1:D:40:LEU:HD23	2.49	0.41
1:B:225:THR:HG21	1:B:252:LEU:HD22	2.02	0.41
1:D:268:ILE:HD11	1:D:275:LEU:HD21	2.03	0.41
1:A:332:ILE:HD13	1:A:332:ILE:HA	1.96	0.41
1:D:122:ASN:HB2	1:D:123:PRO:CD	2.51	0.41
1:A:26:THR:HA	1:A:27:PRO:C	2.46	0.41
1:A:95:VAL:HG11	1:A:108[B]:VAL:HG11	2.03	0.40
1:A:189:PRO:HG3	1:A:224:MET:HE1	2.04	0.40
1:B:320:GLU:HB3	4:B:401:EDO:H12	2.04	0.40
1:D:289:LYS:CG	4:D:402[A]:EDO:H11	2.50	0.40
1:C:52:GLU:O	1:C:85:PRO:HD2	2.21	0.40
1:D:208:ALA:HA	1:D:239:TYR:O	2.22	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	363/381 (95%)	356 (98%)	7 (2%)	0	100	100
1	B	362/381 (95%)	356 (98%)	6 (2%)	0	100	100
1	C	362/381 (95%)	355 (98%)	7 (2%)	0	100	100
1	D	359/381 (94%)	351 (98%)	8 (2%)	0	100	100
All	All	1446/1524 (95%)	1418 (98%)	28 (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	289/331 (87%)	282 (98%)	7 (2%)	43	38
1	B	294/331 (89%)	290 (99%)	4 (1%)	59	59
1	C	283/331 (86%)	275 (97%)	8 (3%)	38	32
1	D	287/331 (87%)	285 (99%)	2 (1%)	76	78
All	All	1153/1324 (87%)	1132 (98%)	21 (2%)	53	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	65	PRO
1	A	128	GLU
1	A	135	SER
1	A	200	THR
1	A	250	LEU
1	A	363	SER
1	B	67	VAL
1	B	114	ILE
1	B	174[A]	THR

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Mol	Chain	Res	Type
1	B	174[B]	THR
1	C	16	VAL
1	C	67	VAL
1	C	95	VAL
1	C	115	ASP
1	C	174	THR
1	C	247[A]	GLU
1	C	247[B]	GLU
1	C	359	VAL
1	D	114	ILE
1	D	229	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	ASN
1	A	324	GLN
1	B	60	HIS
1	C	176	ASN
1	C	278	ASN
1	D	35	ASN
1	D	288	ASN
1	D	306	ASN
1	D	324	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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	EDO	D	402[A]	-	3,3,3	0.38	0	2,2,2	0.45	0
4	EDO	A	404[A]	-	3,3,3	0.41	0	2,2,2	0.28	0
4	EDO	A	403	-	3,3,3	0.50	0	2,2,2	0.32	0
4	EDO	C	405	-	3,3,3	0.87	0	2,2,2	0.09	0
4	EDO	D	402[B]	-	3,3,3	0.63	0	2,2,2	0.32	0
4	EDO	C	403	-	3,3,3	0.47	0	2,2,2	0.27	0
4	EDO	A	405	-	3,3,3	0.50	0	2,2,2	0.21	0
4	EDO	B	401	-	3,3,3	0.97	0	2,2,2	1.13	0
4	EDO	D	403	-	3,3,3	0.27	0	2,2,2	0.78	0
4	EDO	A	404[B]	-	3,3,3	0.32	0	2,2,2	0.74	0
4	EDO	C	404	-	3,3,3	0.73	0	2,2,2	0.21	0
4	EDO	C	406	-	3,3,3	0.29	0	2,2,2	0.57	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	EDO	D	402[A]	-	-	1/1/1/1	-
4	EDO	A	404[A]	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	C	405	-	-	1/1/1/1	-
4	EDO	D	402[B]	-	-	0/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	B	401	-	-	1/1/1/1	-
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	A	404[B]	-	-	0/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	405	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	B	401	EDO	O1-C1-C2-O2
4	D	402[A]	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402[A]	EDO	7	0
4	C	405	EDO	4	0
4	D	402[B]	EDO	4	0
4	B	401	EDO	6	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	361/381 (94%)	1.38	75 (20%) 2 2	17, 26, 37, 46	6 (1%)
1	B	360/381 (94%)	0.81	25 (6%) 23 24	14, 26, 37, 58	6 (1%)
1	C	361/381 (94%)	1.64	116 (32%) 1 1	18, 27, 38, 54	5 (1%)
1	D	361/381 (94%)	0.90	41 (11%) 10 10	14, 27, 38, 56	2 (0%)
All	All	1443/1524 (94%)	1.18	257 (17%) 4 3	14, 26, 38, 58	19 (1%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	ILE	5.0
1	C	14	LEU	4.9
1	C	6	LYS	4.9
1	B	95	VAL	4.7
1	B	100	LYS	4.5
1	A	310	SER	4.4
1	C	96	PHE	4.4
1	C	125	ILE	4.3
1	C	8[A]	THR	4.3
1	B	243	GLY	4.3
1	B	101	ILE	4.2
1	C	5	VAL	4.2
1	C	95	VAL	4.2
1	C	287	TYR	4.2
1	A	292	LEU	4.2
1	C	98	LEU	4.2
1	A	285	ALA	4.1
1	B	363	SER	4.1
1	A	311	TYR	4.0
1	A	307	PHE	4.0
1	B	96	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	93	PHE	4.0
1	A	287	TYR	4.0
1	C	176	ASN	3.9
1	C	316	PHE	3.9
1	D	98	LEU	3.9
1	A	304	CYS	3.9
1	D	295	VAL	3.9
1	A	315	LEU	3.8
1	A	363	SER	3.8
1	C	97	SER	3.8
1	D	291	SER	3.7
1	D	244	GLY	3.7
1	A	1	MET	3.7
1	A	295	VAL	3.7
1	A	319	GLY	3.7
1	C	10	GLY	3.7
1	B	99	PRO	3.6
1	A	291	SER	3.6
1	D	114	ILE	3.6
1	A	281	LEU	3.6
1	D	101	ILE	3.5
1	A	314	HIS	3.5
1	A	312	ILE	3.5
1	C	9	PHE	3.5
1	C	99	PRO	3.5
1	C	67	VAL	3.5
1	C	102	ARG	3.4
1	C	123	PRO	3.4
1	C	174	THR	3.4
1	C	146	VAL	3.4
1	B	98	LEU	3.4
1	A	33	GLY	3.4
1	A	290[A]	ARG	3.4
1	C	285	ALA	3.3
1	A	316	PHE	3.3
1	D	96	PHE	3.3
1	A	326	LEU	3.3
1	D	99	PRO	3.3
1	C	68	GLU	3.3
1	C	118	LYS	3.2
1	A	146	VAL	3.2
1	A	288	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	9	PHE	3.2
1	C	269	ALA	3.2
1	D	100	LYS	3.1
1	C	281	LEU	3.1
1	B	156	GLU	3.1
1	A	299	CYS	3.1
1	C	149	ALA	3.1
1	C	298	ARG	3.1
1	A	286	SER	3.1
1	C	271	HIS	3.1
1	A	301	CYS	3.1
1	A	321	VAL	3.0
1	C	7	LYS	3.0
1	D	146	VAL	3.0
1	A	190	ASP	3.0
1	C	66	GLY	3.0
1	B	93	PHE	3.0
1	B	264	PHE	3.0
1	D	149	ALA	3.0
1	C	24	VAL	2.9
1	D	8[A]	THR	2.9
1	C	1	MET	2.9
1	C	100	LYS	2.9
1	A	302	TYR	2.9
1	A	308	THR	2.9
1	D	304	CYS	2.9
1	A	317	ASP	2.9
1	D	95	VAL	2.9
1	C	59	PHE	2.9
1	C	120	PHE	2.9
1	C	94	GLN	2.9
1	A	166	LEU	2.9
1	C	72	LEU	2.9
1	C	283	LEU	2.9
1	C	315	LEU	2.9
1	B	244	GLY	2.9
1	A	162	TYR	2.8
1	C	151	TYR	2.8
1	C	20	HIS	2.8
1	C	23	ALA	2.8
1	C	310	SER	2.8
1	D	277	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	102	ARG	2.8
1	A	6	LYS	2.8
1	C	350	THR	2.8
1	C	359	VAL	2.8
1	B	292	LEU	2.8
1	C	114	ILE	2.8
1	C	187	ILE	2.7
1	C	268	ILE	2.7
1	C	245	SER	2.7
1	C	264	PHE	2.7
1	B	115	ASP	2.7
1	A	322	LEU	2.7
1	C	313	HIS	2.7
1	C	349	GLY	2.7
1	D	243	GLY	2.7
1	C	89	ASP	2.7
1	A	318	ARG	2.7
1	C	111	ARG	2.7
1	A	283	LEU	2.7
1	C	19	LEU	2.7
1	C	166	LEU	2.7
1	C	286	SER	2.7
1	A	294	PRO	2.6
1	A	114	ILE	2.6
1	A	323	GLY	2.6
1	C	115	ASP	2.6
1	C	317	ASP	2.6
1	A	289	LYS	2.6
1	A	306	ASN	2.6
1	D	69	ILE	2.6
1	C	290	ARG	2.6
1	C	108[A]	VAL	2.6
1	C	348[A]	SER	2.6
1	D	363	SER	2.6
1	C	110	PHE	2.6
1	D	93	PHE	2.6
1	A	5	VAL	2.6
1	C	132	ALA	2.6
1	B	287	TYR	2.5
1	C	75	GLY	2.5
1	C	319	GLY	2.5
1	D	70	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	103	ILE	2.5
1	B	34	THR	2.5
1	D	298	ARG	2.5
1	A	268	ILE	2.5
1	C	69	ILE	2.5
1	C	314	HIS	2.5
1	A	58	THR	2.5
1	D	6	LYS	2.5
1	A	14	LEU	2.5
1	A	231	PHE	2.5
1	A	149	ALA	2.5
1	B	146	VAL	2.5
1	C	119	VAL	2.5
1	C	351	PHE	2.4
1	A	293	GLU	2.4
1	C	295	VAL	2.4
1	D	102	ARG	2.4
1	A	244	GLY	2.4
1	A	320	GLU	2.4
1	A	197	LEU	2.4
1	C	312	ILE	2.4
1	A	50	GLY	2.4
1	A	313	HIS	2.4
1	A	191	LEU	2.4
1	A	199	LEU	2.4
1	C	170	LYS	2.4
1	A	325	ILE	2.4
1	C	318	ARG	2.4
1	C	346	ILE	2.4
1	A	94	GLN	2.4
1	A	57[A]	ASN	2.4
1	C	21	HIS	2.4
1	C	60	HIS	2.4
1	C	16	VAL	2.4
1	C	136	ASP	2.3
1	C	12	ALA	2.3
1	C	342	VAL	2.3
1	C	356	SER	2.3
1	A	44	ARG	2.3
1	B	304	CYS	2.3
1	A	327	LEU	2.3
1	C	212	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	288	ASN	2.3
1	C	131	ILE	2.3
1	B	190	ASP	2.3
1	B	301	CYS	2.3
1	C	34	THR	2.3
1	D	1	MET	2.3
1	C	70	ILE	2.3
1	C	345[A]	SER	2.3
1	A	303	THR	2.3
1	A	298	ARG	2.2
1	A	272	GLY	2.2
1	C	171	ALA	2.2
1	C	62	MET	2.2
1	D	308	THR	2.2
1	D	9	PHE	2.2
1	D	131	ILE	2.2
1	A	309	ARG	2.2
1	D	115	ASP	2.2
1	C	157	ALA	2.2
1	C	57	ASN	2.2
1	D	293	GLU	2.2
1	D	108	VAL	2.2
1	C	235	ASP	2.2
1	D	292	LEU	2.2
1	D	285	ALA	2.2
1	D	94	GLN	2.1
1	A	276	THR	2.1
1	C	121	LEU	2.1
1	B	278	ASN	2.1
1	C	278	ASN	2.1
1	D	356	SER	2.1
1	C	289	LYS	2.1
1	C	17	MET	2.1
1	B	59	PHE	2.1
1	A	151	TYR	2.1
1	C	150	ASP	2.1
1	C	214	ILE	2.1
1	D	125	ILE	2.1
1	C	291	SER	2.1
1	C	134	GLY	2.1
1	C	244	GLY	2.1
1	A	220	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	2.1
1	C	61	LEU	2.1
1	C	76	LEU	2.1
1	C	292	LEU	2.1
1	C	205	ASP	2.1
1	A	101	ILE	2.0
1	A	332	ILE	2.0
1	C	3	PHE	2.0
1	D	334	PHE	2.0
1	A	245	SER	2.0
1	A	350	THR	2.0
1	A	203	GLY	2.0
1	C	282	ASN	2.0
1	D	294	PRO	2.0
1	C	164	TRP	2.0
1	A	51	ALA	2.0
1	C	309	ARG	2.0
1	A	2	GLU	2.0
1	B	291	SER	2.0
1	C	103	ILE	2.0
1	D	264	PHE	2.0
1	C	107	GLY	2.0
1	C	294	PRO	2.0
1	D	113	PRO	2.0
1	C	358	VAL	2.0
1	D	67	VAL	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	EDO	A	403	4/4	0.66	0.25	46,46,47,48	0
4	EDO	C	403	4/4	0.70	0.24	45,46,47,48	0
4	EDO	A	405	4/4	0.76	0.21	46,47,47,47	0
4	EDO	A	404[A]	4/4	0.83	0.15	39,41,41,44	2
4	EDO	A	404[B]	4/4	0.83	0.15	41,41,42,44	2
4	EDO	C	404	4/4	0.84	0.23	30,33,34,34	0
4	EDO	D	402[A]	4/4	0.87	0.32	26,28,28,30	2
4	EDO	D	402[B]	4/4	0.87	0.32	23,25,26,28	2
4	EDO	D	403	4/4	0.88	0.18	33,35,36,36	0
4	EDO	C	406	4/4	0.92	0.14	35,39,39,41	0
4	EDO	B	401	4/4	0.92	0.22	11,12,20,22	0
3	CL	C	402	1/1	0.94	0.11	34,34,34,34	0
3	CL	D	401	1/1	0.95	0.23	26,26,26,26	0
3	CL	A	401	1/1	0.96	0.26	22,22,22,22	0
2	ZN	D	400	1/1	0.97	0.13	29,29,29,29	0
4	EDO	C	405	4/4	0.97	0.22	9,11,14,18	0
3	CL	C	401	1/1	0.98	0.18	17,17,17,17	0
2	ZN	A	400	1/1	0.98	0.14	16,16,16,16	0
3	CL	A	402	1/1	0.98	0.19	19,19,19,19	0
2	ZN	B	400	1/1	0.99	0.14	17,17,17,17	0
2	ZN	C	400	1/1	0.99	0.13	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.