



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:34 PM UTC

PDB ID : 3ITK / pdb_00003itk
Title : Crystal structure of human UDP-glucose dehydrogenase Thr131Ala, apo form.
Authors : Chaikuad, A.; Egger, S.; Yue, W.W.; Sethi, R.; Filippakopoulos, P.; Muniz, J.R.C.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.M.; Kavanagh, K.L.; Nidetzky, B.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2009-08-28
Resolution : 2.40 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

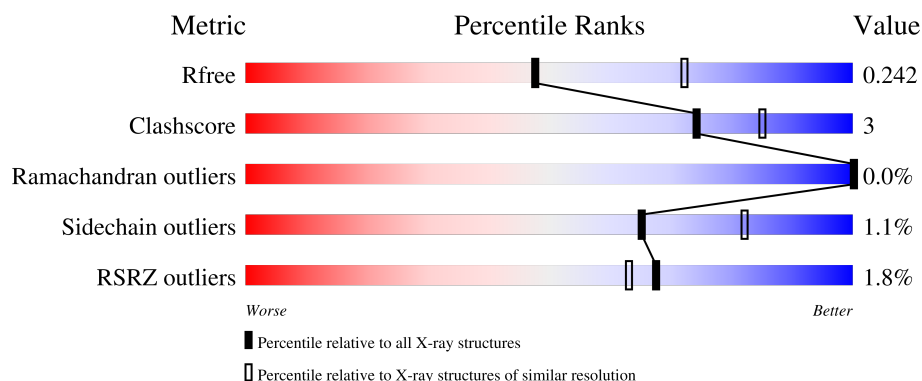
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	467	% 94% 5% .
1	B	467	5% 92% 7% ..
1	C	467	% 94% 6%
1	D	467	% 93% 7%

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Mol	Chain	Length	Quality of chain
1	E	467	% 94%6%
1	F	467	% 89%10%•

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22977 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 UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3591	2277	615	680	19			
1	B	462	Total	C	N	O	S	0	2	0
			3586	2270	615	681	20			
1	C	467	Total	C	N	O	S	0	1	0
			3629	2297	625	688	19			
1	D	467	Total	C	N	O	S	0	0	0
			3622	2295	622	685	20			
1	E	466	Total	C	N	O	S	0	2	0
			3604	2284	619	682	19			
1	F	467	Total	C	N	O	S	0	0	0
			3624	2290	625	690	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O60701
A	131	ALA	THR	engineered mutation	UNP O60701
B	0	SER	-	expression tag	UNP O60701
B	131	ALA	THR	engineered mutation	UNP O60701
C	0	SER	-	expression tag	UNP O60701
C	131	ALA	THR	engineered mutation	UNP O60701
D	0	SER	-	expression tag	UNP O60701
D	131	ALA	THR	engineered mutation	UNP O60701
E	0	SER	-	expression tag	UNP O60701
E	131	ALA	THR	engineered mutation	UNP O60701
F	0	SER	-	expression tag	UNP O60701
F	131	ALA	THR	engineered mutation	UNP O60701

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		
2	D	1	Total	C	O	0	0
			13	8	5		
2	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	211	Total O 211 211	0	0
4	B	171	Total O 171 171	0	0
4	C	215	Total O 215 215	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	202	Total 202	O 202	0	0
4	E	174	Total 174	O 174	0	0
4	F	215	Total 215	O 215	0	0

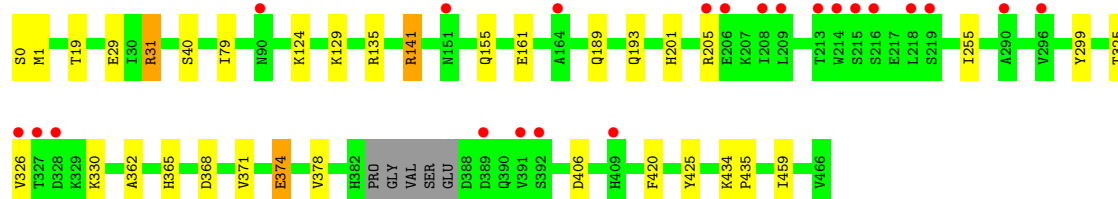
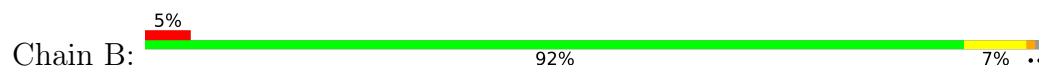
3 Residue-property plots [i](#)

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.

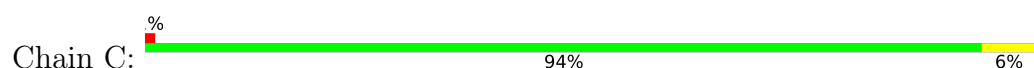
- Molecule 1: UDP-glucose 6-dehydrogenase



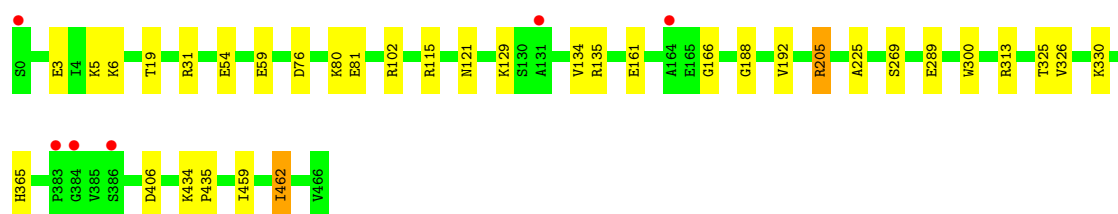
- Molecule 1: UDP-glucose 6-dehydrogenase



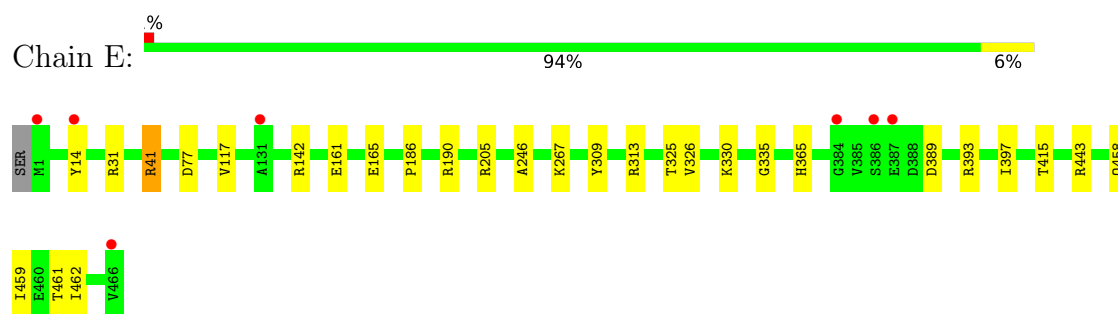
- Molecule 1: UDP-glucose 6-dehydrogenase



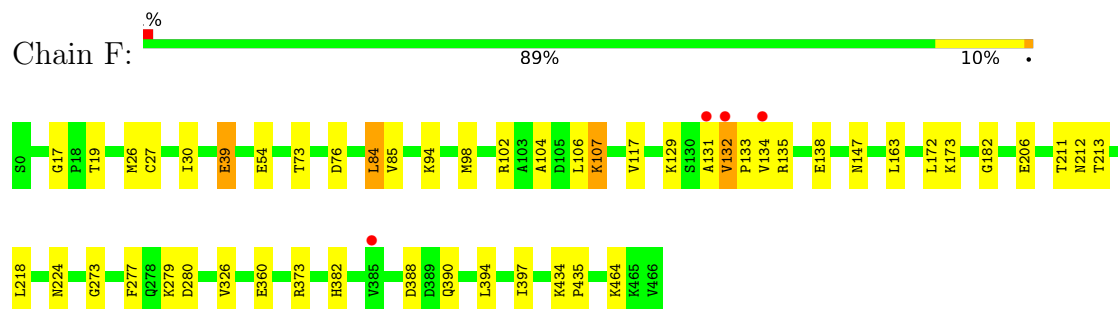
- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.06Å 106.61Å 349.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.90 – 2.40 52.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.90-2.40) 99.7 (52.90-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.198 , 0.241 0.199 , 0.242	Depositor DCC
R_{free} test set	2134 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22977	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: PG4, 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	0.90	2/3657 (0.1%)	0.89	4/4956 (0.1%)
1	B	0.90	1/3656 (0.0%)	1.00	8/4953 (0.2%)
1	C	0.91	2/3699 (0.1%)	0.89	3/5012 (0.1%)
1	D	0.92	3/3689 (0.1%)	0.93	4/4998 (0.1%)
1	E	0.87	1/3676 (0.0%)	0.88	5/4984 (0.1%)
1	F	0.92	0/3691	0.96	4/5003 (0.1%)
All	All	0.90	9/22068 (0.0%)	0.93	28/29906 (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
1	E	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	ARG	CZ-NH1	-11.40	1.16	1.32
1	D	121	ASN	CG-ND2	-8.54	1.15	1.33
1	C	240	LEU	C-O	-7.28	1.15	1.24
1	D	121	ASN	CG-OD1	-7.03	1.10	1.23
1	C	31	ARG	CZ-NH1	-6.11	1.24	1.32
1	A	31	ARG	CZ-NH1	-5.89	1.24	1.32
1	E	31	ARG	CZ-NH1	-5.65	1.24	1.32
1	D	31	ARG	CZ-NH1	-5.64	1.24	1.32
1	A	227	LEU	C-O	-5.61	1.17	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	NE-CZ-NH2	23.40	140.26	119.20
1	B	31	ARG	NE-CZ-NH1	-18.16	103.33	121.50
1	D	205	ARG	CD-NE-CZ	13.42	143.18	124.40
1	D	205	ARG	NE-CZ-NH2	-11.04	109.26	119.20
1	E	41	ARG	CD-NE-CZ	9.06	137.09	124.40
1	B	31	ARG	NH1-CZ-NH2	-7.57	109.47	119.30
1	B	31	ARG	CG-CD-NE	-7.38	95.76	112.00
1	A	31	ARG	NE-CZ-NH2	6.99	125.50	119.20
1	E	31	ARG	NE-CZ-NH2	6.42	124.97	119.20
1	C	31	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	D	80	LYS	N-CA-C	6.01	118.32	111.11
1	E	205	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	D	31	ARG	NE-CZ-NH2	5.76	124.38	119.20
1	C	205	ARG	NE-CZ-NH2	5.65	124.29	119.20
1	B	205	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	C	205	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	E	41	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	E	205	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	B	299	TYR	N-CA-C	-5.38	105.33	111.14
1	B	255	ILE	CB-CA-C	-5.36	105.11	111.97
1	A	255	ILE	CB-CA-C	-5.36	105.00	112.02
1	A	205	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	F	54	GLU	CB-CA-C	-5.30	103.11	110.16
1	A	205	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	F	76	ASP	N-CA-C	5.21	116.96	111.28
1	B	205	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	F	17	GLY	CA-C-N	5.16	124.34	118.97
1	F	17	GLY	C-N-CA	5.16	124.34	118.97

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	31	ARG	Sidechain
1	D	205	ARG	Sidechain
1	E	41	ARG	Sidechain

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	3591	0	3566	14	0
1	B	3586	0	3562	21	1
1	C	3629	0	3611	12	1
1	D	3622	0	3613	22	0
1	E	3604	0	3576	14	0
1	F	3624	0	3595	43	0
2	A	13	0	18	4	0
2	C	26	0	36	4	0
2	D	13	0	18	2	0
2	F	13	0	18	5	0
3	A	4	0	6	0	0
3	B	16	0	24	0	0
3	C	4	0	6	0	0
3	D	20	0	30	0	0
3	E	12	0	18	0	0
3	F	12	0	18	0	0
4	A	211	0	0	6	0
4	B	171	0	0	4	0
4	C	215	0	0	2	0
4	D	202	0	0	4	0
4	E	174	0	0	3	0
4	F	215	0	0	3	0
All	All	22977	0	21715	134	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 3.

All (134) 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)
2:D:467:PG4:O3	2:D:467:PG4:H72	1.65	0.93
1:B:326:VAL:HG11	1:B:362:ALA:HB2	1.53	0.90
1:B:326:VAL:CG1	1:B:362:ALA:HB2	2.10	0.81
1:B:374:GLU:O	1:B:378:VAL:HG23	1.81	0.80
1:F:326:VAL:CG1	1:F:360:GLU:HB3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:MET:HE3	1:F:173:LYS:HG2	1.62	0.79
1:F:326:VAL:HG13	1:F:360:GLU:HB3	1.68	0.76
2:D:467:PG4:O3	2:D:467:PG4:C7	2.34	0.75
1:F:277:PHE:HE2	2:F:467:PG4:H32	1.53	0.74
2:A:467:PG4:C7	2:A:467:PG4:O3	2.36	0.72
1:F:117:VAL:HG21	1:F:147:ASN:HB3	1.74	0.69
1:F:104:ALA:HB3	1:F:133:PRO:HB3	1.75	0.69
1:D:313:ARG:HD2	4:D:1180:HOH:O	1.94	0.68
1:F:326:VAL:CG1	1:F:360:GLU:CB	2.71	0.67
1:F:326:VAL:HG13	1:F:360:GLU:CB	2.24	0.67
1:F:163:LEU:HD21	1:F:172:LEU:HD21	1.81	0.62
1:A:313:ARG:HD2	4:A:992:HOH:O	1.99	0.61
1:B:29:GLU:OE1	1:B:201:HIS:NE2	2.30	0.61
1:C:313:ARG:HD2	4:C:1179:HOH:O	1.99	0.60
1:F:163:LEU:HD21	1:F:172:LEU:HD11	1.82	0.60
1:A:458:GLN:NE2	4:A:479:HOH:O	2.32	0.60
1:C:441:GLY:HA2	1:C:462:ILE:HD12	1.83	0.60
1:D:225:ALA:HB1	1:D:300:TRP:CZ3	2.37	0.60
1:F:132:VAL:HB	1:F:133:PRO:CD	2.33	0.58
1:D:19:THR:HG21	1:D:129:LYS:HE2	1.86	0.58
1:D:102:ARG:NH1	1:D:289:GLU:OE1	2.37	0.58
1:D:330:LYS:HE3	1:D:365:HIS:CE1	2.40	0.57
1:F:273:GLY:H	2:F:467:PG4:H22	1.70	0.56
1:F:182:GLY:HA2	1:F:213:THR:HG22	1.88	0.55
1:B:155:GLN:OE1	4:B:683:HOH:O	2.18	0.55
1:F:27:CYS:HB3	1:F:30:ILE:HD12	1.87	0.54
1:F:84:LEU:C	1:F:84:LEU:HD13	2.33	0.54
1:B:135:ARG:HA	4:B:472:HOH:O	2.07	0.54
1:F:211:THR:HG23	1:F:212:ASN:O	2.07	0.54
1:F:373:ARG:NH1	4:F:484:HOH:O	2.40	0.54
1:A:31:ARG:HD3	4:A:491:HOH:O	2.07	0.53
1:D:313:ARG:CD	4:D:1180:HOH:O	2.54	0.53
1:A:29:GLU:OE1	1:A:201:HIS:NE2	2.33	0.52
1:A:313:ARG:NH1	4:A:992:HOH:O	1.94	0.52
1:C:277:PHE:HE2	2:C:467:PG4:H22	1.75	0.52
1:F:135:ARG:HA	1:F:138:GLU:OE2	2.10	0.52
1:F:19:THR:HG21	1:F:129:LYS:HE3	1.91	0.52
1:F:277:PHE:CE2	2:F:467:PG4:H32	2.39	0.52
1:C:0:SER:O	1:C:1:MET:HB3	2.10	0.51
1:F:39:GLU:HG3	1:F:73:THR:HG21	1.92	0.51
1:C:281:VAL:O	1:C:285:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:THR:HG23	1:D:325:THR:O	2.11	0.50
1:C:443:ARG:HD3	1:C:462:ILE:O	2.12	0.49
1:E:77:ASP:HB3	4:E:1026:HOH:O	2.13	0.49
1:E:14:TYR:OH	1:E:165:GLU:HA	2.12	0.49
1:F:106:LEU:O	1:F:107:LYS:C	2.56	0.48
1:B:325:THR:O	1:B:325:THR:HG23	2.13	0.48
1:F:224:ASN:ND2	1:F:280:ASP:OD2	2.47	0.48
1:A:434:LYS:HA	1:A:435:PRO:C	2.37	0.48
1:C:330:LYS:HE3	1:C:365:HIS:CE1	2.48	0.48
4:C:528:HOH:O	1:E:142:ARG:CD	2.62	0.48
1:F:382:HIS:ND1	1:F:388:ASP:OD1	2.45	0.48
1:E:330:LYS:HE3	1:E:365:HIS:CE1	2.49	0.47
2:C:467:PG4:H42	2:C:467:PG4:H11	1.96	0.47
1:E:335:GLY:HA3	1:E:415:THR:HB	1.95	0.47
1:D:102:ARG:HD3	4:D:511:HOH:O	2.15	0.47
1:D:330:LYS:NZ	1:D:406:ASP:O	2.43	0.47
1:B:374:GLU:HB2	4:B:1154:HOH:O	2.14	0.47
1:F:132:VAL:CB	1:F:133:PRO:CD	2.93	0.47
1:E:458:GLN:NE2	4:E:498:HOH:O	2.35	0.47
1:F:26:MET:CE	1:F:173:LYS:HG2	2.38	0.47
1:D:134:VAL:O	1:D:135:ARG:HB2	2.15	0.46
1:B:330:LYS:HE3	1:B:365:HIS:CE1	2.50	0.46
2:C:467:PG4:H42	2:C:467:PG4:C1	2.46	0.46
1:E:389:ASP:O	1:E:393:ARG:HB2	2.14	0.46
1:B:141[A]:ARG:NH1	4:B:533:HOH:O	2.48	0.46
1:F:84:LEU:C	1:F:84:LEU:CD1	2.89	0.46
1:A:330:LYS:HE3	1:A:365:HIS:CE1	2.51	0.46
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.52	0.45
1:C:434:LYS:HA	1:C:435:PRO:C	2.41	0.45
1:E:246:ALA:CB	1:F:218:LEU:HD23	2.45	0.45
1:F:132:VAL:O	1:F:133:PRO:C	2.60	0.45
1:C:189:GLN:O	1:C:193:GLN:HG2	2.16	0.45
2:C:467:PG4:C1	2:C:467:PG4:C4	2.95	0.45
1:D:269:SER:C	1:D:462:ILE:HD13	2.41	0.45
1:F:102:ARG:HD2	4:F:884:HOH:O	2.16	0.45
2:A:467:PG4:O3	2:A:467:PG4:H71	2.17	0.45
1:B:326:VAL:CG1	1:B:362:ALA:CB	2.89	0.45
1:D:3:GLU:OE2	1:D:5:LYS:HE3	2.17	0.45
1:F:464:LYS:NZ	4:F:586:HOH:O	2.50	0.45
1:F:390:GLN:HG2	1:F:394:LEU:HD12	1.98	0.44
1:B:19:THR:HG21	1:B:129:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:LEU:HD13	1:F:85:VAL:N	2.33	0.44
1:A:373:ARG:HB2	1:A:397:ILE:HD12	1.99	0.44
1:D:76:ASP:OD1	1:D:115:ARG:NE	2.46	0.44
1:E:186:PRO:O	1:E:190[A]:ARG:HG3	2.17	0.44
1:C:1:MET:O	1:C:1:MET:CG	2.66	0.44
1:E:309:TYR:CZ	1:E:313:ARG:HD3	2.53	0.44
1:F:94:LYS:NZ	1:F:98:MET:O	2.51	0.44
1:C:134:VAL:O	1:C:135:ARG:HB2	2.18	0.44
1:B:0:SER:O	1:B:1:MET:C	2.61	0.43
1:A:330:LYS:HE3	1:A:365:HIS:CD2	2.53	0.43
1:B:79:ILE:O	1:B:124:LYS:HE3	2.17	0.43
1:B:326:VAL:O	1:B:326:VAL:HG12	2.18	0.43
1:A:405:CYS:HB3	1:A:428:ILE:HG23	2.01	0.43
1:F:132:VAL:HB	1:F:133:PRO:HD2	2.00	0.43
1:B:368:ASP:OD1	1:B:371:VAL:HG23	2.19	0.43
1:F:434:LYS:HA	1:F:435:PRO:C	2.42	0.43
1:E:267:LYS:HB3	4:E:912:HOH:O	2.19	0.43
1:F:132:VAL:HG11	1:F:279:LYS:HD3	2.00	0.43
1:F:273:GLY:H	2:F:467:PG4:C2	2.31	0.42
1:C:19:THR:HG21	1:C:129:LYS:HE2	2.01	0.42
1:D:54:GLU:CD	1:D:166:GLY:H	2.26	0.42
1:D:313:ARG:CG	4:D:1180:HOH:O	2.67	0.42
1:F:131:ALA:O	1:F:132:VAL:O	2.37	0.42
1:A:332:ALA:HB2	1:A:404:ALA:O	2.19	0.42
1:B:330:LYS:NZ	1:B:406:ASP:O	2.37	0.42
1:F:134:VAL:O	1:F:135:ARG:HB2	2.20	0.42
1:B:434:LYS:HA	1:B:435:PRO:C	2.45	0.41
1:F:326:VAL:HG13	1:F:360:GLU:HB2	2.00	0.41
2:A:467:PG4:H22	4:A:761:HOH:O	2.21	0.41
1:B:420:PHE:O	1:B:425:TYR:OH	2.36	0.41
2:A:467:PG4:O3	2:A:467:PG4:H72	2.20	0.41
1:D:434:LYS:HA	1:D:435:PRO:C	2.46	0.41
1:F:373:ARG:HB2	1:F:397:ILE:HG21	2.02	0.41
1:A:84:LEU:HD13	1:A:84:LEU:C	2.46	0.41
1:A:393:ARG:NH1	4:A:808:HOH:O	2.54	0.41
1:B:326:VAL:HG12	1:B:362:ALA:CA	2.51	0.41
1:D:6:LYS:HD3	1:D:81:GLU:HB3	2.03	0.41
1:D:59:GLU:N	1:D:59:GLU:CD	2.79	0.41
1:D:188:GLY:O	1:D:192:VAL:HG23	2.20	0.40
1:D:225:ALA:HB1	1:D:300:TRP:CE3	2.56	0.40
1:D:326:VAL:O	1:D:326:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:GLY:N	2:F:467:PG4:H22	2.36	0.40
1:D:59:GLU:CD	1:D:59:GLU:H	2.29	0.40
1:E:325:THR:O	1:E:325:THR:HG23	2.20	0.40
1:E:443:ARG:HD3	1:E:462:ILE:O	2.21	0.40
1:E:443:ARG:HD2	1:E:461:THR:OG1	2.22	0.40
1:B:189:GLN:O	1:B:193:GLN:HG2	2.21	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)
1:B:40:SER:OG	1:C:77:ASP:OD1[1_455]	1.82	0.38

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	460/467 (98%)	449 (98%)	11 (2%)	0	100	100
1	B	460/467 (98%)	447 (97%)	13 (3%)	0	100	100
1	C	466/467 (100%)	453 (97%)	13 (3%)	0	100	100
1	D	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	E	466/467 (100%)	454 (97%)	12 (3%)	0	100	100
1	F	465/467 (100%)	446 (96%)	18 (4%)	1 (0%)	43	58
All	All	2782/2802 (99%)	2704 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	132	VAL

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	385/400 (96%)	380 (99%)	5 (1%)	61	80
1	B	386/400 (96%)	381 (99%)	5 (1%)	61	80
1	C	391/400 (98%)	387 (99%)	4 (1%)	68	84
1	D	391/400 (98%)	388 (99%)	3 (1%)	73	86
1	E	385/400 (96%)	380 (99%)	5 (1%)	61	80
1	F	391/400 (98%)	387 (99%)	4 (1%)	68	84
All	All	2329/2400 (97%)	2303 (99%)	26 (1%)	65	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	161	GLU
1	A	326	VAL
1	A	370	LYS
1	A	449	HIS
1	B	141[A]	ARG
1	B	141[B]	ARG
1	B	161	GLU
1	B	374	GLU
1	B	459	ILE
1	C	161	GLU
1	C	170	LYS
1	C	184	GLU
1	C	326	VAL
1	D	161	GLU
1	D	459	ILE
1	D	462	ILE
1	E	117	VAL
1	E	161	GLU
1	E	326	VAL
1	E	397	ILE
1	E	459	ILE

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Mol	Chain	Res	Type
1	F	39	GLU
1	F	84	LEU
1	F	107	LYS
1	F	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	193	GLN
1	A	302	GLN
1	B	155	GLN
1	B	159	ASN
1	B	193	GLN
1	B	302	GLN
1	C	151	ASN
1	C	155	GLN
1	C	193	GLN
1	C	363	HIS
1	C	458	GLN
1	D	302	GLN
1	D	390	GLN
1	E	155	GLN
1	E	174	ASN
1	E	193	GLN
1	E	302	GLN
1	F	292	ASN
1	F	390	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

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	$\# Z > 2$
3	EDO	D	470	-	3,3,3	0.52	0	2,2,2	0.69	0
3	EDO	C	469	-	3,3,3	0.60	0	2,2,2	0.15	0
3	EDO	D	471	-	3,3,3	0.57	0	2,2,2	0.19	0
3	EDO	F	470	-	3,3,3	0.55	0	2,2,2	0.36	0
3	EDO	F	468	-	3,3,3	0.50	0	2,2,2	0.21	0
3	EDO	B	467	-	3,3,3	0.56	0	2,2,2	0.20	0
2	PG4	C	468	-	12,12,12	0.48	0	11,11,11	0.45	0
2	PG4	C	467	-	12,12,12	0.62	0	11,11,11	0.87	0
3	EDO	D	468	-	3,3,3	0.69	0	2,2,2	0.22	0
3	EDO	D	469	-	3,3,3	0.51	0	2,2,2	0.36	0
3	EDO	A	468	-	3,3,3	0.61	0	2,2,2	0.13	0
3	EDO	F	469	-	3,3,3	0.63	0	2,2,2	0.25	0
3	EDO	E	467	-	3,3,3	0.65	0	2,2,2	0.04	0
2	PG4	F	467	-	12,12,12	0.67	0	11,11,11	0.84	0
3	EDO	B	469	-	3,3,3	0.44	0	2,2,2	0.54	0
2	PG4	A	467	-	12,12,12	0.53	0	11,11,11	0.58	0
3	EDO	E	469	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	B	470	-	3,3,3	0.53	0	2,2,2	0.16	0
3	EDO	E	468	-	3,3,3	0.67	0	2,2,2	0.13	0
2	PG4	D	467	-	12,12,12	0.83	0	11,11,11	1.05	0
3	EDO	B	468	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	D	472	-	3,3,3	0.50	0	2,2,2	0.26	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
3	EDO	D	470	-	-	0/1/1/1	-
3	EDO	C	469	-	-	0/1/1/1	-
3	EDO	D	471	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	F	470	-	-	0/1/1/1	-
3	EDO	F	468	-	-	1/1/1/1	-
3	EDO	B	467	-	-	1/1/1/1	-
2	PG4	C	468	-	-	6/10/10/10	-
2	PG4	C	467	-	-	7/10/10/10	-
3	EDO	D	468	-	-	1/1/1/1	-
3	EDO	D	469	-	-	0/1/1/1	-
3	EDO	A	468	-	-	1/1/1/1	-
3	EDO	F	469	-	-	1/1/1/1	-
3	EDO	E	467	-	-	1/1/1/1	-
2	PG4	F	467	-	-	6/10/10/10	-
3	EDO	B	469	-	-	0/1/1/1	-
2	PG4	A	467	-	-	7/10/10/10	-
3	EDO	E	469	-	-	0/1/1/1	-
3	EDO	B	470	-	-	1/1/1/1	-
3	EDO	E	468	-	-	1/1/1/1	-
2	PG4	D	467	-	-	7/10/10/10	-
3	EDO	B	468	-	-	1/1/1/1	-
3	EDO	D	472	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	467	PG4	C5-C6-O4-C7
2	F	467	PG4	C3-C4-O3-C5
2	C	467	PG4	C1-C2-O2-C3
2	D	467	PG4	C1-C2-O2-C3
2	F	467	PG4	O3-C5-C6-O4
2	C	467	PG4	C4-C3-O2-C2
2	F	467	PG4	C4-C3-O2-C2
2	A	467	PG4	O2-C3-C4-O3
2	C	467	PG4	O2-C3-C4-O3
2	A	467	PG4	O4-C7-C8-O5
2	C	467	PG4	O1-C1-C2-O2
3	E	467	EDO	O1-C1-C2-O2
3	F	468	EDO	O1-C1-C2-O2
2	D	467	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
2	C	467	PG4	O3-C5-C6-O4
2	A	467	PG4	O3-C5-C6-O4
2	D	467	PG4	O3-C5-C6-O4
2	C	468	PG4	O4-C7-C8-O5
2	C	468	PG4	O3-C5-C6-O4
2	C	468	PG4	C3-C4-O3-C5
3	B	470	EDO	O1-C1-C2-O2
2	D	467	PG4	O4-C7-C8-O5
2	F	467	PG4	O1-C1-C2-O2
2	D	467	PG4	O2-C3-C4-O3
2	A	467	PG4	C5-C6-O4-C7
3	D	471	EDO	O1-C1-C2-O2
3	F	469	EDO	O1-C1-C2-O2
2	C	467	PG4	C6-C5-O3-C4
2	A	467	PG4	C8-C7-O4-C6
3	A	468	EDO	O1-C1-C2-O2
2	C	468	PG4	C5-C6-O4-C7
2	C	468	PG4	C8-C7-O4-C6
3	B	468	EDO	O1-C1-C2-O2
2	F	467	PG4	O2-C3-C4-O3
3	D	468	EDO	O1-C1-C2-O2
3	D	472	EDO	O1-C1-C2-O2
2	D	467	PG4	O1-C1-C2-O2
2	A	467	PG4	C3-C4-O3-C5
3	B	467	EDO	O1-C1-C2-O2
3	E	468	EDO	O1-C1-C2-O2
2	F	467	PG4	C6-C5-O3-C4
2	A	467	PG4	C4-C3-O2-C2
2	C	468	PG4	O2-C3-C4-O3
2	C	467	PG4	C8-C7-O4-C6

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	467	PG4	4	0
2	F	467	PG4	5	0
2	A	467	PG4	4	0
2	D	467	PG4	2	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	A	464/467 (99%)	-0.52	6 (1%) 75 71	2, 13, 32, 52	0
1	B	462/467 (98%)	0.09	22 (4%) 35 32	3, 13, 32, 58	2 (0%)
1	C	467/467 (100%)	-0.52	5 (1%) 78 74	2, 13, 32, 68	1 (0%)
1	D	467/467 (100%)	-0.43	6 (1%) 75 71	3, 13, 32, 65	0
1	E	466/467 (99%)	-0.32	7 (1%) 72 68	2, 13, 32, 64	2 (0%)
1	F	467/467 (100%)	-0.52	4 (0%) 81 78	3, 13, 32, 64	0
All	All	2793/2802 (99%)	-0.37	50 (1%) 67 63	2, 13, 32, 68	5 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	SER	4.7
1	B	213	THR	4.2
1	C	1	MET	4.2
1	A	1	MET	3.8
1	B	389	ASP	3.8
1	A	0	SER	3.4
1	F	131	ALA	3.3
1	D	0	SER	3.1
1	D	164	ALA	3.0
1	E	14	TYR	3.0
1	B	215	SER	3.0
1	B	326	VAL	2.9
1	F	132	VAL	2.9
1	B	164	ALA	2.9
1	B	214	TRP	2.9
1	D	386	SER	2.9
1	F	134	VAL	2.8
1	E	1	MET	2.6
1	B	409	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	131	ALA	2.6
1	B	206	GLU	2.6
1	E	384	GLY	2.6
1	E	387	GLU	2.6
1	B	328	ASP	2.5
1	A	387	GLU	2.5
1	D	383	PRO	2.5
1	B	218	LEU	2.5
1	B	327	THR	2.5
1	B	209	LEU	2.4
1	B	290	ALA	2.4
1	B	219	SER	2.4
1	C	14	TYR	2.4
1	E	466	VAL	2.4
1	A	164	ALA	2.3
1	B	216	SER	2.3
1	B	90	ASN	2.3
1	A	383	PRO	2.3
1	E	386	SER	2.3
1	F	385	VAL	2.3
1	B	151	ASN	2.2
1	B	205	ARG	2.2
1	C	384	GLY	2.2
1	B	391	VAL	2.2
1	B	392	SER	2.1
1	A	165	GLU	2.1
1	B	296	VAL	2.0
1	D	131	ALA	2.0
1	D	384	GLY	2.0
1	B	208	ILE	2.0
1	C	383	PRO	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
3	EDO	D	470	4/4	0.56	0.25	43,56,58,63	0
3	EDO	B	467	4/4	0.68	0.24	58,59,59,65	0
3	EDO	F	470	4/4	0.73	0.18	52,53,55,60	0
3	EDO	C	469	4/4	0.75	0.18	55,63,65,67	0
3	EDO	E	468	4/4	0.77	0.25	49,54,55,61	0
2	PG4	F	467	13/13	0.79	0.17	30,47,61,67	0
3	EDO	D	472	4/4	0.81	0.24	62,64,66,70	0
3	EDO	B	469	4/4	0.81	0.20	29,51,56,60	0
3	EDO	D	469	4/4	0.81	0.17	60,63,69,69	0
3	EDO	B	468	4/4	0.82	0.23	52,59,63,64	0
2	PG4	D	467	13/13	0.82	0.18	27,44,51,55	0
3	EDO	F	468	4/4	0.83	0.22	36,47,55,57	0
3	EDO	D	471	4/4	0.84	0.17	39,49,49,53	0
3	EDO	F	469	4/4	0.86	0.15	39,45,49,51	0
3	EDO	E	469	4/4	0.88	0.15	49,50,54,56	0
3	EDO	B	470	4/4	0.88	0.21	38,54,55,57	0
2	PG4	C	468	13/13	0.89	0.12	23,49,59,64	0
3	EDO	A	468	4/4	0.89	0.15	32,39,44,48	0
3	EDO	E	467	4/4	0.90	0.19	32,37,37,38	0
2	PG4	C	467	13/13	0.90	0.15	26,42,49,49	0
3	EDO	D	468	4/4	0.90	0.12	38,39,41,42	0
2	PG4	A	467	13/13	0.92	0.11	17,36,51,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.