Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 05:24 PM EST

PDB ID	:	5MKV
Title	:	Crystal Structure of Human Dihydropyrimidinease-like 2 (DPYSL2A)/Collapsin Response Mediator Protein (CRMP2) residues 13-516
Authors	:	Sethi, R.; Zheng, Y.; Krojer, T.; Velupillai, S.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Ahmed, A.A.; von Delft, F.
Deposited on	:	2016-12-05
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

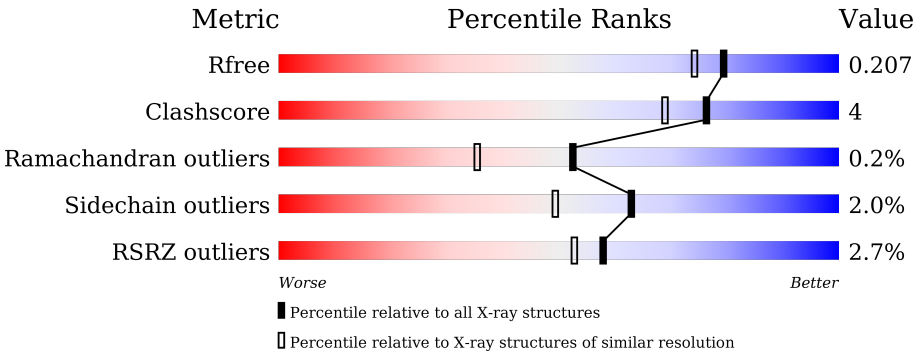
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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 <=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	504	88% 8%
1	B	504	3% 85% 9%
1	C	504	2% 89% 8%
1	D	504	4% 87% 10%

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
2	EDO	A	601	-	-	-	X
2	EDO	A	602	-	-	-	X
2	EDO	A	603	-	-	-	X
2	EDO	A	604	-	-	-	X
2	EDO	A	605	-	-	-	X
2	EDO	A	606	-	-	X	X
2	EDO	A	607	-	-	X	X
2	EDO	A	609	-	-	-	X
2	EDO	A	610	-	-	-	X
2	EDO	A	611	-	-	-	X
2	EDO	B	601	-	-	-	X
2	EDO	B	602	-	-	-	X
2	EDO	B	603	-	-	X	X
2	EDO	B	604	-	-	X	X
2	EDO	C	601	-	-	-	X
2	EDO	D	602	-	-	-	X
2	EDO	D	603	-	-	-	X
2	EDO	D	605	-	-	-	X
2	EDO	D	606	-	-	-	X

2 Entry composition

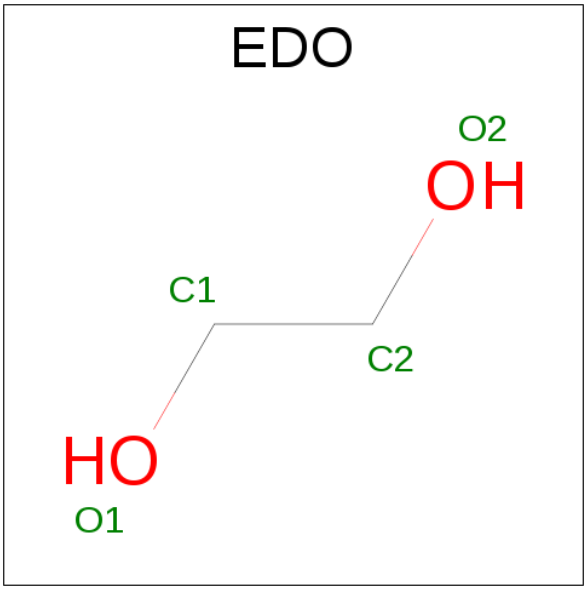
There are 3 unique types of molecules in this entry. The entry contains 15644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydropyrimidinase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3732	2352	638	724	18			
1	B	482	Total	C	N	O	S	0	1	0
			3704	2334	634	717	19			
1	C	493	Total	C	N	O	S	0	0	0
			3781	2382	645	735	19			
1	D	488	Total	C	N	O	S	0	0	0
			3743	2358	640	726	19			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 3 is water.

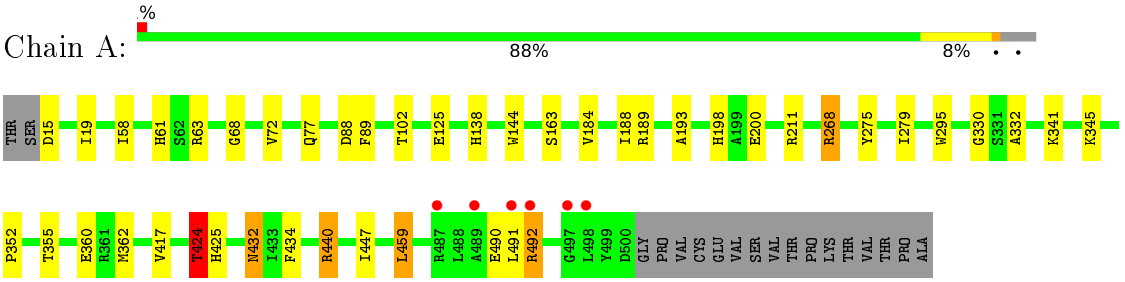
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	220	Total O 220 220	0	0
3	B	84	Total O 84 84	0	0
3	C	154	Total O 154 154	0	0
3	D	138	Total O 138 138	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

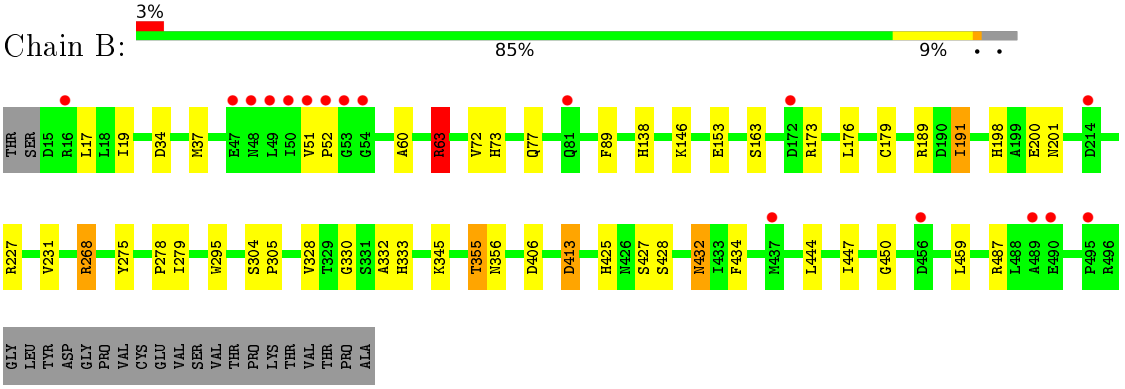
- Molecule 1: Dihydropyrimidinase-related protein 2

Chain A:



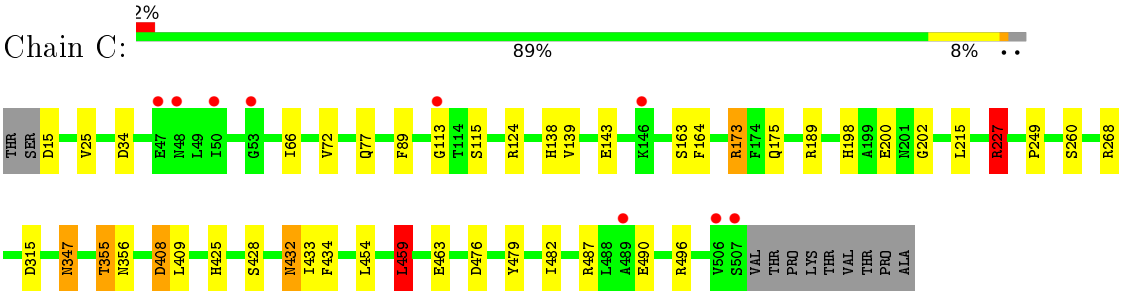
- Molecule 1: Dihydropyrimidinase-related protein 2

Chain B:



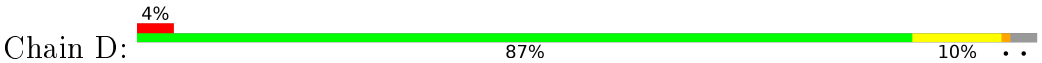
- Molecule 1: Dihydropyrimidinase-related protein 2

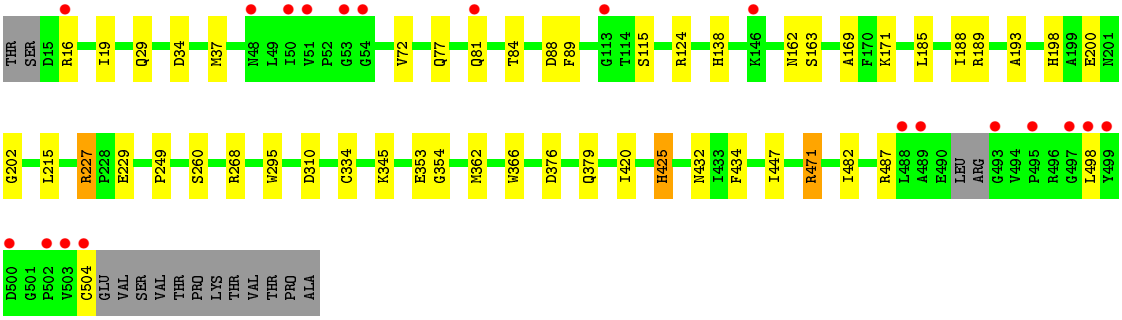
Chain C:



- Molecule 1: Dihydropyrimidinase-related protein 2

Chain D:




THR SER D15 R16 I19 Q29 D34 M37 N48 L49 I50 V51 P52 G53 G54 V72 Q77 Q81 T84 D88 F89 G113 T114 S115 R124 H138 K146 N162 S163 A169 F170 K171 L185 I188 R189 A193 H198 A199 E200 N201
G202 L215 R227 P228 E229 P249 S260 R268 W295 D310 C334 K345 E353 G354 M362 W366 D376 Q379 I420 H425 N432 I433 F434 I447 R471 I482 R487 L488 A489 E490 LEU ARG G493 V494 P495 R496 G497 L498 Y499
D500 G501 P502 V503 C504 GLU VAL SER VAL THR PRO LYS THR VAL THR PRO ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.90Å 157.51Å 87.42Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	19.87 – 1.80 19.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.87-1.80) 97.8 (19.87-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.167 , 0.200 0.177 , 0.207	Depositor DCC
R_{free} test set	9717 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15644	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	1.02	5/3809 (0.1%)	1.02	8/5171 (0.2%)
1	B	0.93	0/3783	0.99	12/5135 (0.2%)
1	C	1.04	4/3859 (0.1%)	1.19	20/5240 (0.4%)
1	D	0.98	5/3820 (0.1%)	1.10	15/5185 (0.3%)
All	All	0.99	14/15271 (0.1%)	1.08	55/20731 (0.3%)

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	C	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	ARG	CD-NE	-9.98	1.29	1.46
1	C	260	SER	CB-OG	-9.97	1.29	1.42
1	D	362	MET	CG-SD	-6.83	1.63	1.81
1	D	227	ARG	CD-NE	-6.72	1.35	1.46
1	A	125	GLU	CD-OE1	-6.48	1.18	1.25
1	D	229	GLU	CD-OE1	6.41	1.32	1.25
1	A	362	MET	CG-SD	-6.34	1.64	1.81
1	D	353	GLU	CD-OE2	-6.32	1.18	1.25
1	C	490	GLU	CG-CD	5.74	1.60	1.51
1	C	463	GLU	CD-OE2	-5.46	1.19	1.25
1	A	424	THR	CB-CG2	-5.27	1.34	1.52
1	A	362	MET	CB-CG	5.24	1.68	1.51
1	D	260	SER	CB-OG	-5.14	1.35	1.42
1	A	360	GLU	CD-OE1	5.04	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	227	ARG	NE-CZ-NH2	-35.50	102.55	120.30
1	D	227	ARG	NE-CZ-NH2	-28.93	105.84	120.30
1	C	227	ARG	NE-CZ-NH1	23.35	131.97	120.30
1	D	227	ARG	NE-CZ-NH1	18.40	129.50	120.30
1	D	268	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	C	268	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	A	268	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	B	227	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	B	227	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	C	487	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	A	268	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	D	487	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	C	227	ARG	CD-NE-CZ	8.32	135.25	123.60
1	B	268	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	487	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	189	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	173	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	487	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	315	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	268	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	C	189	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	487	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	424	THR	N-CA-CB	-6.61	97.75	110.30
1	C	173	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	268	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	227	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	34	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	189	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	D	268	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	496	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	34	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	173	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	88	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	227	ARG	CG-CD-NE	-5.71	99.81	111.80
1	C	227	ARG	CG-CD-NE	-5.70	99.83	111.80
1	D	189	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	471	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	C	124	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	406	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	496	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	413	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	124	ARG	NE-CZ-NH1	5.55	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	459	LEU	CA-CB-CG	5.54	128.05	115.30
1	D	81	GLN	CA-CB-CG	5.37	125.21	113.40
1	A	63	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	63	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	459	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	34	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	211	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	185	LEU	CB-CG-CD1	5.16	119.76	111.00
1	C	476	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	408	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	58	ILE	CB-CA-C	-5.03	101.54	111.60
1	D	124	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	310	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	227	ARG	Sidechain

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	3732	0	3667	28	0
1	B	3704	0	3647	37	0
1	C	3781	0	3712	21	0
1	D	3743	0	3677	23	0
2	A	44	0	66	9	0
2	B	16	0	24	14	0
2	C	4	0	6	0	0
2	D	24	0	36	6	0
3	A	220	0	0	5	0
3	B	84	0	0	5	0
3	C	154	0	0	3	0
3	D	138	0	0	2	0
All	All	15644	0	14835	114	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 (114) 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:A:606:EDO:H21	3:A:710:HOH:O	1.58	1.01
1:B:268:ARG:HE	2:B:603:EDO:C1	1.81	0.93
1:A:332:ALA:O	2:A:606:EDO:H12	1.75	0.87
1:A:77:GLN:HE21	1:A:89:PHE:H	1.27	0.80
1:A:432:ASN:HD22	1:A:434:PHE:H	1.30	0.79
1:B:138:HIS:HD2	1:B:163:SER:OG	1.65	0.78
1:D:425:HIS:HB2	2:D:606:EDO:H11	1.66	0.77
1:A:424:THR:HG21	3:A:734:HOH:O	1.85	0.76
2:B:604:EDO:H22	3:B:724:HOH:O	1.88	0.74
1:C:432:ASN:HD22	1:C:434:PHE:H	1.35	0.73
1:A:332:ALA:O	2:A:606:EDO:C1	2.37	0.73
1:C:113:GLY:N	1:C:143:GLU:OE2	2.20	0.72
1:D:77:GLN:HE21	1:D:89:PHE:H	1.37	0.71
1:A:15:ASP:N	3:A:701:HOH:O	2.23	0.70
1:C:200:GLU:OE2	1:C:227:ARG:HD3	1.92	0.69
1:C:138:HIS:HD2	1:C:163:SER:OG	1.76	0.67
1:C:355:THR:HG23	1:C:356:ASN:O	1.93	0.67
1:B:268:ARG:NE	2:B:603:EDO:O1	2.27	0.66
1:B:432:ASN:HD22	1:B:434:PHE:H	1.43	0.65
1:B:17:LEU:HD23	1:B:37:MET:HE1	1.80	0.64
1:C:198:HIS:HD2	3:C:832:HOH:O	1.80	0.64
1:D:138:HIS:HD2	1:D:163:SER:OG	1.81	0.64
2:B:602:EDO:O1	3:B:702:HOH:O	2.15	0.63
1:A:198:HIS:HD2	3:A:892:HOH:O	1.82	0.62
1:D:366:TRP:HZ2	2:D:604:EDO:H12	1.65	0.62
1:A:138:HIS:HD2	1:A:163:SER:OG	1.84	0.61
1:B:198:HIS:HD2	3:B:771:HOH:O	1.82	0.61
1:B:37:MET:HE1	1:B:447:ILE:HG21	1.84	0.59
1:D:198:HIS:HD2	3:D:827:HOH:O	1.85	0.59
1:B:153:GLU:CG	1:B:191:ILE:HD11	2.33	0.58
1:D:200:GLU:OE2	1:D:227:ARG:HD3	2.04	0.57
1:A:198:HIS:HE1	1:A:200:GLU:OE1	1.87	0.57
1:B:153:GLU:HG2	1:B:191:ILE:HD11	1.86	0.56
1:B:333:HIS:HE1	2:B:604:EDO:H22	1.70	0.56
1:B:17:LEU:HD23	1:B:37:MET:CE	2.35	0.56
1:B:37:MET:HE3	1:B:450:GLY:HA2	1.86	0.56
1:C:198:HIS:HE1	1:C:200:GLU:OE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:LEU:HD13	1:C:459:LEU:HD13	1.88	0.56
1:B:268:ARG:HE	2:B:603:EDO:H12	1.67	0.55
1:B:268:ARG:NE	2:B:603:EDO:C1	2.62	0.55
1:B:427:SER:HB2	2:B:604:EDO:H21	1.89	0.55
2:D:603:EDO:H22	3:D:819:HOH:O	2.05	0.55
1:B:19:ILE:HD11	1:B:447:ILE:HD13	1.88	0.55
1:C:249:PRO:HB3	1:C:482:ILE:HD11	1.90	0.54
1:D:366:TRP:CZ2	2:D:604:EDO:H12	2.42	0.54
1:C:347:ASN:C	1:C:347:ASN:HD22	2.11	0.54
1:D:249:PRO:HB3	1:D:482:ILE:HD11	1.89	0.54
1:B:77:GLN:HE21	1:B:89:PHE:H	1.57	0.53
1:D:425:HIS:HB2	2:D:606:EDO:C1	2.37	0.53
1:C:479:TYR:HA	1:C:482:ILE:HD12	1.90	0.53
1:A:355:THR:OG1	2:A:606:EDO:H22	2.07	0.53
1:B:201:ASN:HB3	1:B:231:VAL:HG13	1.91	0.52
1:A:19:ILE:HD11	1:A:447:ILE:CD1	2.40	0.52
1:B:198:HIS:HE1	1:B:200:GLU:OE1	1.93	0.52
1:B:179[B]:CYS:SG	1:D:171:LYS:NZ	2.76	0.50
1:D:162:ASN:OD1	1:D:471:ARG:NH1	2.43	0.50
1:C:25:VAL:HB	1:C:66:ILE:HG22	1.94	0.50
1:C:432:ASN:ND2	1:C:434:PHE:H	2.07	0.50
1:A:432:ASN:ND2	1:A:434:PHE:H	2.03	0.50
1:A:268:ARG:HH22	2:A:607:EDO:H12	1.75	0.50
1:A:72:VAL:O	1:A:138:HIS:HE1	1.96	0.49
1:C:408:ASP:C	1:C:409:LEU:HD12	2.33	0.48
1:D:72:VAL:O	1:D:138:HIS:HE1	1.96	0.48
1:D:198:HIS:HE1	1:D:200:GLU:OE1	1.96	0.48
1:A:77:GLN:NE2	1:A:88:ASP:HB2	2.29	0.48
1:A:492:ARG:CB	3:C:818:HOH:O	2.62	0.48
1:C:77:GLN:HE21	1:C:89:PHE:H	1.60	0.48
1:D:376:ASP:H	1:D:379:GLN:NE2	2.12	0.47
1:A:417:VAL:HG22	1:A:440:ARG:HG3	1.97	0.47
1:C:138:HIS:CD2	1:C:163:SER:OG	2.64	0.47
1:B:279:ILE:HA	1:B:330:GLY:O	2.15	0.46
1:C:72:VAL:O	1:C:138:HIS:HE1	1.98	0.46
1:B:432:ASN:ND2	1:B:434:PHE:H	2.13	0.46
1:B:275:TYR:CE1	2:B:603:EDO:C2	3.00	0.45
1:B:60:ALA:O	1:B:63:ARG:HB2	2.15	0.45
1:A:268:ARG:NH2	2:A:607:EDO:H12	2.32	0.45
1:D:420:ILE:HG21	1:D:434:PHE:HB2	1.99	0.45
1:C:139:VAL:O	1:C:164:PHE:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HH22	2:A:607:EDO:H21	1.82	0.44
1:B:304:SER:HA	1:B:305:PRO:C	2.37	0.44
1:B:37:MET:CE	1:B:447:ILE:HG21	2.48	0.44
1:A:279:ILE:HA	1:A:330:GLY:O	2.18	0.44
1:B:413:ASP:HB2	1:B:444:LEU:HG	2.00	0.43
1:B:275:TYR:CE1	2:B:603:EDO:H22	2.53	0.43
1:A:275:TYR:HE1	2:A:607:EDO:H11	1.83	0.43
1:C:175:GLN:OE1	1:C:202:GLY:HA3	2.19	0.43
1:C:77:GLN:HG2	3:C:704:HOH:O	2.18	0.43
1:D:334:CYS:O	1:D:354:GLY:HA3	2.19	0.43
1:B:72:VAL:O	1:B:138:HIS:HE1	2.02	0.43
1:B:153:GLU:HG3	1:B:191:ILE:HD11	1.99	0.42
1:D:295:TRP:CZ2	1:D:345:LYS:HA	2.54	0.42
1:A:355:THR:H	2:A:606:EDO:C1	2.32	0.42
1:B:355:THR:HG23	1:B:356:ASN:O	2.19	0.42
1:B:51:VAL:HG12	1:B:52:PRO:O	2.20	0.42
2:B:601:EDO:C1	3:B:703:HOH:O	2.68	0.42
1:B:73:HIS:CD2	1:B:332:ALA:HA	2.55	0.42
1:D:188:ILE:HG23	1:D:193:ALA:HB3	2.02	0.42
1:B:278:PRO:HD2	1:B:328:VAL:O	2.19	0.41
1:A:61:HIS:HE1	3:A:909:HOH:O	2.02	0.41
1:D:169:ALA:HA	1:D:202:GLY:HA3	2.02	0.41
1:B:275:TYR:CE1	2:B:603:EDO:H21	2.55	0.41
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.55	0.41
1:A:68:GLY:HA3	1:A:102:THR:OG1	2.21	0.41
2:B:604:EDO:C2	3:B:724:HOH:O	2.58	0.41
1:D:432:ASN:ND2	2:D:606:EDO:H21	2.36	0.41
1:B:295:TRP:CZ2	1:B:345:LYS:HA	2.56	0.41
1:B:268:ARG:NE	2:B:603:EDO:H12	2.33	0.41
1:D:19:ILE:HD11	1:D:447:ILE:CD1	2.51	0.41
1:D:249:PRO:HD3	1:D:482:ILE:HD13	2.03	0.41
1:A:341:LYS:HA	1:A:352:PRO:HD2	2.02	0.40
1:A:144:TRP:CE3	1:A:184:VAL:HG22	2.57	0.40
1:A:188:ILE:HG23	1:A:193:ALA:HB3	2.04	0.40
1:C:355:THR:OG1	1:C:433:ILE:HG21	2.21	0.40
1:D:376:ASP:H	1:D:379:GLN:HE21	1.70	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	484/504 (96%)	469 (97%)	13 (3%)	2 (0%)	39	23
1	B	481/504 (95%)	465 (97%)	15 (3%)	1 (0%)	52	35
1	C	491/504 (97%)	481 (98%)	10 (2%)	0	100	100
1	D	484/504 (96%)	468 (97%)	16 (3%)	0	100	100
All	All	1940/2016 (96%)	1883 (97%)	54 (3%)	3 (0%)	52	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	GLU
1	A	492	ARG
1	B	146	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/423 (96%)	398 (98%)	6 (2%)	72	62
1	B	402/423 (95%)	394 (98%)	8 (2%)	63	49
1	C	410/423 (97%)	400 (98%)	10 (2%)	57	41
1	D	406/423 (96%)	397 (98%)	9 (2%)	60	45
All	All	1622/1692 (96%)	1589 (98%)	33 (2%)	63	49

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	424	THR
1	A	425	HIS
1	A	432	ASN
1	A	440	ARG
1	A	459	LEU
1	A	491	LEU
1	B	63	ARG
1	B	176	LEU
1	B	191	ILE
1	B	355	THR
1	B	425	HIS
1	B	428	SER
1	B	432	ASN
1	B	459	LEU
1	C	15	ASP
1	C	115	SER
1	C	173	ARG
1	C	215	LEU
1	C	347	ASN
1	C	355	THR
1	C	425	HIS
1	C	428	SER
1	C	432	ASN
1	C	459	LEU
1	D	16	ARG
1	D	29	GLN
1	D	37	MET
1	D	84	THR
1	D	115	SER
1	D	215	LEU
1	D	425	HIS
1	D	498	LEU
1	D	504	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	61	HIS
1	A	77	GLN
1	A	138	HIS
1	A	198	HIS
1	A	209	GLN

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Mol	Chain	Res	Type
1	A	245	GLN
1	A	426	ASN
1	A	432	ASN
1	B	77	GLN
1	B	91	GLN
1	B	122	GLN
1	B	138	HIS
1	B	149	GLN
1	B	198	HIS
1	B	266	GLN
1	B	426	ASN
1	B	432	ASN
1	C	77	GLN
1	C	138	HIS
1	C	149	GLN
1	C	198	HIS
1	C	209	GLN
1	C	210	GLN
1	C	347	ASN
1	C	432	ASN
1	D	77	GLN
1	D	138	HIS
1	D	198	HIS
1	D	209	GLN
1	D	379	GLN
1	D	426	ASN

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 carbohydrates 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	A	601	-	3,3,3	0.47	0	2,2,2	0.49	0
2	EDO	A	602	-	3,3,3	0.37	0	2,2,2	1.57	0
2	EDO	A	603	-	3,3,3	0.60	0	2,2,2	0.60	0
2	EDO	A	604	-	3,3,3	0.70	0	2,2,2	0.15	0
2	EDO	A	605	-	3,3,3	0.75	0	2,2,2	0.37	0
2	EDO	A	606	-	3,3,3	0.32	0	2,2,2	1.59	1 (50%)
2	EDO	A	607	-	3,3,3	1.04	0	2,2,2	1.14	0
2	EDO	A	608	-	3,3,3	0.34	0	2,2,2	0.53	0
2	EDO	A	609	-	3,3,3	0.79	0	2,2,2	0.46	0
2	EDO	A	610	-	3,3,3	1.55	0	2,2,2	0.67	0
2	EDO	A	611	-	3,3,3	0.49	0	2,2,2	1.10	0
2	EDO	B	601	-	3,3,3	0.47	0	2,2,2	0.97	0
2	EDO	B	602	-	3,3,3	0.31	0	2,2,2	1.36	0
2	EDO	B	603	-	3,3,3	0.96	0	2,2,2	1.00	0
2	EDO	B	604	-	3,3,3	0.48	0	2,2,2	0.49	0
2	EDO	C	601	-	3,3,3	0.69	0	2,2,2	0.77	0
2	EDO	D	601	-	3,3,3	0.60	0	2,2,2	1.26	0
2	EDO	D	602	-	3,3,3	0.50	0	2,2,2	0.50	0
2	EDO	D	603	-	3,3,3	0.50	0	2,2,2	0.26	0
2	EDO	D	604	-	3,3,3	0.91	0	2,2,2	1.25	0
2	EDO	D	605	-	3,3,3	0.45	0	2,2,2	1.33	0
2	EDO	D	606	-	3,3,3	0.74	0	2,2,2	0.93	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	A	601	-	-	0/1/1/1	0/0/0/0
2	EDO	A	602	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	603	-	-	0/1/1/1	0/0/0/0
2	EDO	A	604	-	-	0/1/1/1	0/0/0/0
2	EDO	A	605	-	-	0/1/1/1	0/0/0/0
2	EDO	A	606	-	-	0/1/1/1	0/0/0/0
2	EDO	A	607	-	-	0/1/1/1	0/0/0/0
2	EDO	A	608	-	-	0/1/1/1	0/0/0/0
2	EDO	A	609	-	-	0/1/1/1	0/0/0/0
2	EDO	A	610	-	-	0/1/1/1	0/0/0/0
2	EDO	A	611	-	-	0/1/1/1	0/0/0/0
2	EDO	B	601	-	-	0/1/1/1	0/0/0/0
2	EDO	B	602	-	-	0/1/1/1	0/0/0/0
2	EDO	B	603	-	-	0/1/1/1	0/0/0/0
2	EDO	B	604	-	-	0/1/1/1	0/0/0/0
2	EDO	C	601	-	-	0/1/1/1	0/0/0/0
2	EDO	D	601	-	-	0/1/1/1	0/0/0/0
2	EDO	D	602	-	-	0/1/1/1	0/0/0/0
2	EDO	D	603	-	-	0/1/1/1	0/0/0/0
2	EDO	D	604	-	-	0/1/1/1	0/0/0/0
2	EDO	D	605	-	-	0/1/1/1	0/0/0/0
2	EDO	D	606	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	606	EDO	O2-C2-C1	-2.14	97.61	112.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	606	EDO	5	0
2	A	607	EDO	4	0
2	B	601	EDO	1	0
2	B	602	EDO	1	0
2	B	603	EDO	8	0
2	B	604	EDO	4	0
2	D	603	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	604	EDO	2	0
2	D	606	EDO	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, 95^{th} 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	486/504 (96%)	-0.33	6 (1%) 81 78	12, 19, 36, 79	0
1	B	482/504 (95%)	-0.06	17 (3%) 48 42	16, 27, 48, 69	0
1	C	493/504 (97%)	-0.26	9 (1%) 71 67	13, 21, 38, 65	0
1	D	488/504 (96%)	-0.12	20 (4%) 41 35	15, 24, 51, 86	0
All	All	1949/2016 (96%)	-0.19	52 (2%) 58 53	12, 23, 45, 86	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	LEU	6.4
1	D	498	LEU	6.4
1	D	50	ILE	5.0
1	B	50	ILE	4.9
1	D	500	ASP	4.8
1	C	50	ILE	4.7
1	C	53	GLY	4.6
1	C	507	SER	4.3
1	B	489	ALA	4.3
1	D	497	GLY	4.2
1	D	504	CYS	3.7
1	B	495	PRO	3.7
1	D	146	LYS	3.6
1	D	48	ASN	3.5
1	D	53	GLY	3.5
1	B	54	GLY	3.5
1	C	48	ASN	3.5
1	A	492	ARG	3.4
1	A	489	ALA	3.3
1	D	54	GLY	3.3
1	D	489	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	495	PRO	3.2
1	B	53	GLY	3.1
1	D	81	GLN	3.1
1	B	81	GLN	3.0
1	C	489	ALA	2.9
1	D	499	TYR	2.8
1	D	493	GLY	2.8
1	D	502	PRO	2.8
1	B	49	LEU	2.7
1	A	497	GLY	2.7
1	A	487	ARG	2.7
1	B	52	PRO	2.7
1	B	437	MET	2.6
1	B	51	VAL	2.6
1	B	48	ASN	2.6
1	C	113	GLY	2.6
1	B	172	ASP	2.5
1	B	16	ARG	2.5
1	D	503	VAL	2.4
1	D	113	GLY	2.3
1	B	456	ASP	2.3
1	B	490	GLU	2.3
1	C	47	GLU	2.3
1	D	51	VAL	2.3
1	D	488	LEU	2.3
1	C	506	VAL	2.1
1	A	498	LEU	2.1
1	B	47	GLU	2.1
1	D	16	ARG	2.0
1	B	214	ASP	2.0
1	C	146	LYS	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	EDO	A	609	4/4	0.62	0.22	20.35	49,51,53,56	0
2	EDO	A	610	4/4	0.61	0.28	19.46	36,36,40,46	0
2	EDO	A	606	4/4	0.94	0.27	14.39	38,39,40,45	0
2	EDO	B	604	4/4	0.87	0.33	14.38	35,52,54,65	0
2	EDO	D	606	4/4	0.92	0.27	11.44	26,35,36,39	0
2	EDO	D	603	4/4	0.81	0.33	11.39	34,35,45,48	0
2	EDO	B	603	4/4	0.78	0.22	9.62	27,36,37,40	0
2	EDO	A	607	4/4	0.72	0.20	9.09	37,39,45,47	0
2	EDO	B	601	4/4	0.85	0.26	8.85	32,33,35,43	0
2	EDO	A	611	4/4	0.78	0.19	6.40	41,44,47,53	0
2	EDO	D	602	4/4	0.88	0.22	5.97	34,35,35,35	0
2	EDO	C	601	4/4	0.84	0.15	4.93	34,36,38,39	0
2	EDO	B	602	4/4	0.85	0.20	4.83	42,43,49,52	0
2	EDO	A	601	4/4	0.90	0.13	4.17	34,39,44,51	0
2	EDO	A	603	4/4	0.90	0.18	4.17	34,43,49,52	0
2	EDO	A	602	4/4	0.86	0.17	4.01	42,49,51,57	0
2	EDO	A	605	4/4	0.81	0.16	3.65	40,41,44,50	0
2	EDO	D	605	4/4	0.87	0.20	2.88	40,45,45,46	0
2	EDO	A	604	4/4	0.90	0.18	2.30	39,43,45,46	0
2	EDO	D	604	4/4	0.81	0.17	1.96	28,31,36,42	0
2	EDO	D	601	4/4	0.88	0.18	1.73	31,34,35,35	0
2	EDO	A	608	4/4	0.95	0.11	1.21	32,38,40,41	0

6.5 Other polymers

There are no such residues in this entry.