



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:19 AM UTC

PDB ID : 8PJE / pdb_00008pje
Title : Human Leukocyte Antigen class II allotype DR1 presenting influenza A virus haemagglutinin (HA)306-318 PKYVKQNTLKLAT
Authors : MacLachlan, B.J.; Wall, A.; Greenshields-Watson, A.L.; Hesketh, S.J.; Cole, D.K.; Rizkallah, P.J.; Godkin, A.J.
Deposited on : 2023-06-23
Resolution : 1.70 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

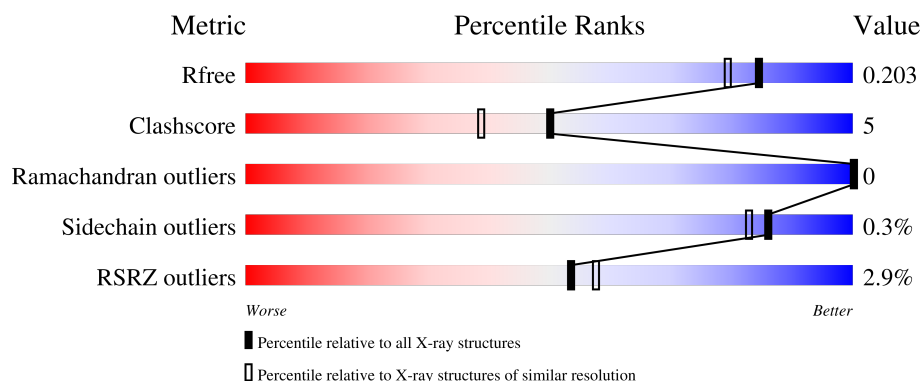
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	186	2% 85% 10%
1	D	186	% 84% 12%
2	B	194	4% 90% 8%
2	E	194	5% 90% 10%
3	C	13	85% 15%

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Mol	Chain	Length	Quality of chain
3	F	13	 85% 15%

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
5	EDO	D	202	-	-	X	-
6	GOL	E	208	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7140 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	6	0
			1508	977	248	277	6			
1	D	179	Total	C	N	O	S	0	2	0
			1481	960	239	276	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P01903
A	-2	GLY	-	expression tag	UNP P01903
A	-1	SER	-	expression tag	UNP P01903
A	0	MET	-	expression tag	UNP P01903
D	-3	MET	-	initiating methionine	UNP P01903
D	-2	GLY	-	expression tag	UNP P01903
D	-1	SER	-	expression tag	UNP P01903
D	0	MET	-	expression tag	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	1	0
			1581	992	283	299	7			
2	E	194	Total	C	N	O	S	0	0	0
			1583	994	283	298	8			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	initiating methionine	UNP P01911
B	-2	GLY	-	expression tag	UNP P01911
B	-1	SER	-	expression tag	UNP P01911
B	0	MET	-	expression tag	UNP P01911

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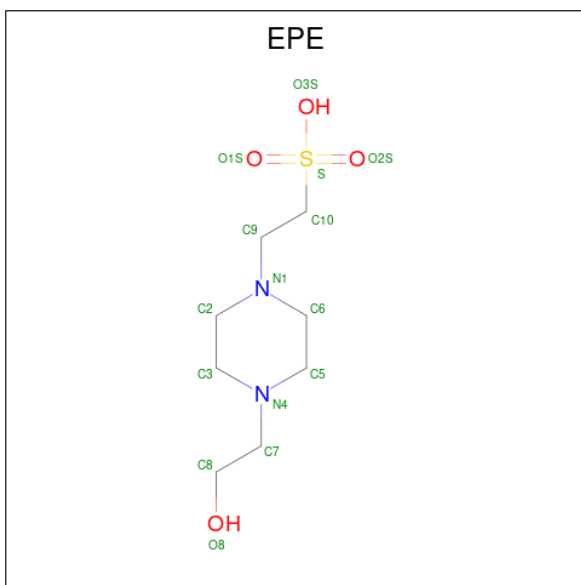
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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	LEU	PRO	variant	UNP P01911
B	13	PHE	ARG	variant	UNP P01911
B	26	LEU	PHE	variant	UNP P01911
B	28	GLU	ASP	variant	UNP P01911
B	30	CYS	TYR	variant	UNP P01911
B	31	ILE	PHE	variant	UNP P01911
B	47	TYR	PHE	variant	UNP P01911
B	67	LEU	ILE	variant	UNP P01911
B	71	ARG	ALA	variant	UNP P01911
B	86	GLY	VAL	variant	UNP P01911
B	96	GLU	GLN	variant	UNP P01911
B	133	ARG	LEU	variant	UNP P01911
B	142	VAL	MET	variant	UNP P01911
E	-3	MET	-	initiating methionine	UNP P01911
E	-2	GLY	-	expression tag	UNP P01911
E	-1	SER	-	expression tag	UNP P01911
E	0	MET	-	expression tag	UNP P01911
E	11	LEU	PRO	variant	UNP P01911
E	13	PHE	ARG	variant	UNP P01911
E	26	LEU	PHE	variant	UNP P01911
E	28	GLU	ASP	variant	UNP P01911
E	30	CYS	TYR	variant	UNP P01911
E	31	ILE	PHE	variant	UNP P01911
E	47	TYR	PHE	variant	UNP P01911
E	67	LEU	ILE	variant	UNP P01911
E	71	ARG	ALA	variant	UNP P01911
E	86	GLY	VAL	variant	UNP P01911
E	96	GLU	GLN	variant	UNP P01911
E	133	ARG	LEU	variant	UNP P01911
E	142	VAL	MET	variant	UNP P01911

- Molecule 3 is a protein called Hemagglutinin.

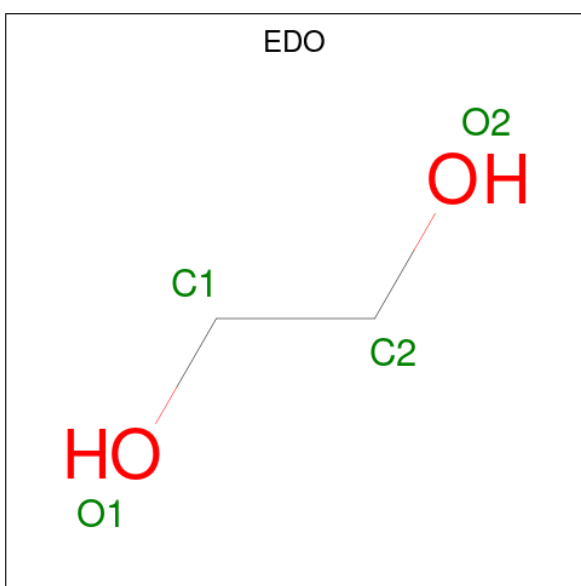
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	F	13	Total	C	N	O	0	0	0
			106	69	18	19			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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



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

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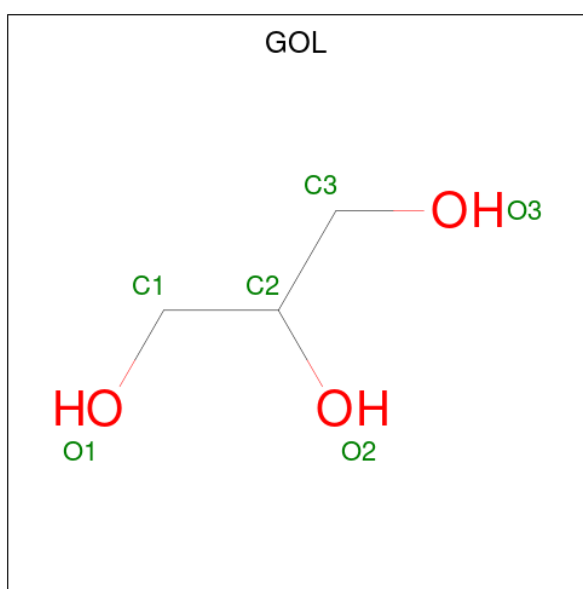
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

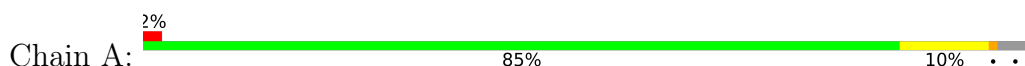
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	152	Total	O	0	0
			152	152		
7	B	133	Total	O	0	0
			133	133		
7	C	11	Total	O	0	0
			11	11		
7	D	154	Total	O	0	0
			154	154		
7	E	112	Total	O	0	0
			112	112		
7	F	9	Total	O	0	0
			9	9		

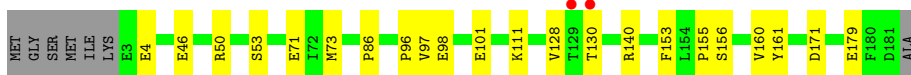
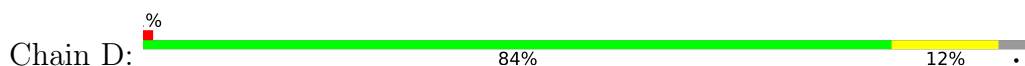
3 Residue-property plots [i](#)

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: HLA class II histocompatibility antigen, DR alpha chain



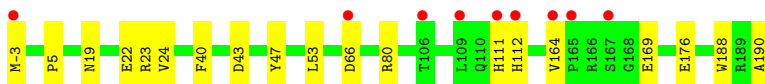
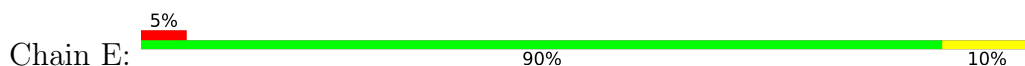
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



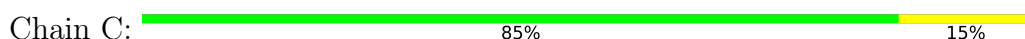
- Molecule 2: HLA class II histocompatibility antigen, DRB1 beta chain



- Molecule 2: HLA class II histocompatibility antigen, DRB1 beta chain



- Molecule 3: Hemagglutinin



- Molecule 3: Hemagglutinin

Chain F:  85% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.50Å 89.18Å 137.44Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	32.81 – 1.70 32.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.81-1.70) 99.5 (32.81-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.203 0.171 , 0.203	Depositor DCC
R_{free} test set	5556 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7140	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, EPE, GOL

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	0.86	0/1571	0.90	2/2138 (0.1%)
1	D	0.81	0/1532	0.83	0/2088
2	B	0.79	0/1621	0.93	7/2199 (0.3%)
2	E	0.79	0/1623	1.03	11/2201 (0.5%)
3	C	0.87	0/107	0.94	0/141
3	F	0.86	0/107	0.91	0/141
All	All	0.81	0/6561	0.93	20/8908 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	66	ASP	CB-CA-C	14.03	133.79	109.24
2	E	111	HIS	CA-C-N	-11.13	104.12	122.82
2	E	111	HIS	C-N-CA	-11.13	104.12	122.82
1	A	50	ARG	CG-CD-NE	-9.84	90.36	112.00
2	B	139	LYS	CA-CB-CG	-8.49	97.11	114.10
2	E	66	ASP	N-CA-CB	-8.22	98.46	110.47
2	B	139	LYS	CG-CD-CE	-6.84	95.56	111.30
2	B	33	ASN	CA-C-N	-6.25	112.85	122.60
2	B	33	ASN	C-N-CA	-6.25	112.85	122.60
2	B	139	LYS	CB-CG-CD	6.24	125.65	111.30
2	E	112	HIS	N-CA-C	-6.04	100.22	109.41
2	E	169	GLU	CA-CB-CG	6.04	126.18	114.10
2	E	66	ASP	N-CA-C	-5.80	106.33	113.41
2	E	112	HIS	CB-CG-CD2	-5.69	123.80	131.20
2	E	66	ASP	OD1-CG-OD2	5.57	136.27	122.90
2	E	176	GLU	CA-CB-CG	-5.42	103.27	114.10
2	E	66	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	128	VAL	CB-CA-C	-5.25	102.85	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	THR	OG1-CB-CG2	-5.19	98.93	109.30
2	B	55	ARG	CB-CG-CD	5.02	122.85	111.30

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	A	1508	0	1465	18	0
1	D	1481	0	1421	19	0
2	B	1581	0	1509	15	0
2	E	1583	0	1514	12	0
3	C	106	0	121	2	0
3	F	106	0	121	1	0
4	A	15	0	17	0	0
4	D	15	0	18	2	0
5	A	20	0	30	6	0
5	B	24	0	36	6	0
5	C	8	0	12	1	0
5	D	24	0	36	8	0
5	E	20	0	30	1	0
5	F	12	0	18	1	0
6	A	12	0	16	2	0
6	B	30	0	39	3	0
6	C	6	0	8	0	0
6	E	18	0	23	5	0
7	A	152	0	0	0	0
7	B	133	0	0	4	0
7	C	11	0	0	0	0
7	D	154	0	0	3	0
7	E	112	0	0	1	0
7	F	9	0	0	0	0
All	All	7140	0	6434	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) 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:B:80:ARG:HH22	6:B:208:GOL:H31	1.24	1.02
2:E:80:ARG:HH12	6:E:208:GOL:H32	1.33	0.91
1:A:160:VAL:HG23	1:A:179:GLU:HG3	1.55	0.89
2:E:19:ASN:ND2	2:E:22:GLU:OE2	2.18	0.76
2:B:106:THR:HG23	2:B:108:PRO:HD3	1.69	0.75
1:D:160:VAL:HG12	1:D:179:GLU:HG3	1.70	0.73
1:A:157:THR:H	5:A:204:EDO:H21	1.53	0.73
5:A:202:EDO:H11	7:D:402:HOH:O	1.90	0.70
1:D:4:GLU:OE2	7:D:301:HOH:O	2.12	0.67
1:D:73:MET:HE1	2:E:53:LEU:HG	1.76	0.67
1:A:28:GLY:O	1:A:146[A]:ARG:NH2	2.26	0.66
1:A:110:ASP:OD1	1:A:146[B]:ARG:HG2	2.00	0.62
2:B:55:ARG:HD2	6:B:211:GOL:H32	1.83	0.60
1:A:134:GLU:O	6:A:208:GOL:H2	2.02	0.60
2:B:75:VAL:HG13	7:B:367:HOH:O	2.02	0.59
1:D:156:SER:N	5:D:202:EDO:H11	2.17	0.58
1:D:161:TYR:HE1	5:D:202:EDO:H21	1.68	0.58
1:D:98:GLU:HB2	1:D:101:GLU:HG3	1.86	0.57
2:B:59:GLU:HG2	5:B:205:EDO:O1	2.06	0.56
1:A:160:VAL:HG23	1:A:179:GLU:CG	2.32	0.56
5:E:203:EDO:H22	7:E:328:HOH:O	2.06	0.56
2:E:80:ARG:HH22	6:E:208:GOL:C1	2.19	0.55
2:B:139:LYS:NZ	5:B:206:EDO:H21	2.22	0.55
1:D:153:PHE:HD2	5:D:202:EDO:H12	1.72	0.54
2:B:94:ARG:NH1	7:B:304:HOH:O	2.41	0.54
1:A:86:PRO:O	5:A:203:EDO:H11	2.07	0.53
1:A:75:LYS:HE3	1:D:71:GLU:OE1	2.08	0.53
2:E:188:TRP:CZ3	2:E:190:ALA:HB2	2.44	0.52
2:E:40:PHE:HB2	2:E:47:TYR:CE2	2.47	0.50
2:B:23:ARG:HH11	2:B:23:ARG:HG2	1.76	0.50
1:D:171:ASP:HB3	2:E:-3:MET:HE1	1.93	0.50
1:A:160:VAL:CG2	1:A:177:HIS:CE1	2.96	0.49
1:D:97:VAL:O	4:D:201:EPE:H101	2.13	0.49
1:D:86:PRO:HD2	5:D:207:EDO:H22	1.94	0.48
1:D:155:PRO:HA	5:D:202:EDO:C1	2.44	0.48
1:D:111:LYS:HG2	1:D:140:ARG:CZ	2.44	0.47
1:A:3:GLU:HG2	1:A:4:GLU:N	2.29	0.47
1:A:157:THR:H	5:A:204:EDO:C2	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:207:GOL:H11	3:C:1:PRO:HD2	1.97	0.47
2:B:99:VAL:HB	5:B:202:EDO:H12	1.95	0.47
1:A:47:GLU:HG2	1:A:48:PHE:N	2.31	0.46
1:A:128:VAL:HG12	1:A:130:THR:HG22	1.99	0.45
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.52	0.45
3:C:9:LEU:HB3	5:C:102:EDO:H22	1.99	0.45
1:A:168:TRP:O	5:A:206:EDO:H11	2.17	0.45
2:E:80:ARG:NH1	6:E:208:GOL:H32	2.16	0.45
1:A:160:VAL:HG22	1:A:177:HIS:CE1	2.51	0.44
4:D:201:EPE:H32	4:D:201:EPE:H82	1.60	0.44
2:E:80:ARG:HH22	6:E:208:GOL:H11	1.82	0.44
1:D:46:GLU:OE2	1:D:50:ARG:NH2	2.48	0.44
5:B:202:EDO:H11	7:B:314:HOH:O	2.16	0.44
5:B:206:EDO:H22	7:B:307:HOH:O	2.17	0.43
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.53	0.43
2:B:139:LYS:HZ2	5:B:206:EDO:H21	1.82	0.43
3:F:12:ALA:HA	5:F:102:EDO:H21	1.99	0.43
2:B:137:GLU:OE2	2:B:139:LYS:HE3	2.18	0.43
5:A:205:EDO:H21	2:E:5:PRO:HG2	2.00	0.43
2:B:87:GLU:O	2:B:92:GLN:HG3	2.19	0.43
1:D:128:VAL:CG2	1:D:130:THR:HG22	2.49	0.42
1:D:53:SER:HB3	5:D:205:EDO:H12	2.00	0.42
1:D:153:PHE:CD2	5:D:202:EDO:H12	2.52	0.42
2:B:18:PHE:HB2	2:B:23:ARG:HB3	2.02	0.41
1:D:96:PRO:O	7:D:302:HOH:O	2.21	0.41
1:A:130:THR:O	1:A:130:THR:HG23	2.20	0.41
2:E:24:VAL:H	6:E:208:GOL:C1	2.33	0.41
2:E:23:ARG:NH2	2:E:43:ASP:OD1	2.47	0.41
1:D:155:PRO:HA	5:D:202:EDO:H11	2.03	0.40
1:A:63:ILE:HA	1:A:63:ILE:HD13	1.89	0.40
1:A:150:TYR:CD1	6:B:209:GOL:H31	2.57	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	A	183/186 (98%)	180 (98%)	3 (2%)	0	100	100
1	D	179/186 (96%)	176 (98%)	3 (2%)	0	100	100
2	B	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
2	E	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	768/786 (98%)	749 (98%)	19 (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	170/169 (101%)	170 (100%)	0	100	100
1	D	166/169 (98%)	166 (100%)	0	100	100
2	B	174/174 (100%)	174 (100%)	0	100	100
2	E	174/174 (100%)	173 (99%)	1 (1%)	78	72
3	C	12/12 (100%)	12 (100%)	0	100	100
3	F	12/12 (100%)	11 (92%)	1 (8%)	10	2
All	All	708/710 (100%)	706 (100%)	2 (0%)	86	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	164	VAL
3	F	1	PRO

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

Mol	Chain	Res	Type
1	A	18	GLN
2	B	92	GLN
2	B	113	ASN
1	D	18	GLN
2	E	112	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 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	$\# Z > 2$
6	GOL	E	208	-	5,5,5	1.35	1 (20%)	5,5,5	0.74	0
5	EDO	B	202	-	3,3,3	0.40	0	2,2,2	0.70	0
5	EDO	B	203	-	3,3,3	0.52	0	2,2,2	0.16	0
5	EDO	E	203	-	3,3,3	0.47	0	2,2,2	0.76	0
5	EDO	D	202	-	3,3,3	0.30	0	2,2,2	1.25	0
5	EDO	C	102	-	3,3,3	0.47	0	2,2,2	0.50	0
6	GOL	B	210	-	5,5,5	1.37	1 (20%)	5,5,5	0.96	0
5	EDO	C	101	-	3,3,3	0.43	0	2,2,2	0.48	0
6	GOL	B	211	-	5,5,5	1.10	1 (20%)	5,5,5	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	E	201	-	3,3,3	0.67	0	2,2,2	0.80	0
6	GOL	B	207	-	5,5,5	1.97	1 (20%)	5,5,5	0.73	0
5	EDO	A	206	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	D	204	-	3,3,3	0.49	0	2,2,2	0.11	0
5	EDO	B	204	-	3,3,3	0.61	0	2,2,2	0.25	0
6	GOL	C	103	-	5,5,5	2.95	3 (60%)	5,5,5	0.62	0
6	GOL	B	208	-	5,5,5	1.09	0	5,5,5	1.09	0
6	GOL	E	206	-	5,5,5	0.85	0	5,5,5	1.05	0
4	EPE	A	201	-	15,15,15	0.90	1 (6%)	19,20,20	2.08	6 (31%)
6	GOL	E	207	-	5,5,5	1.16	0	5,5,5	0.92	0
5	EDO	D	205	-	3,3,3	0.39	0	2,2,2	0.68	0
5	EDO	B	205	-	3,3,3	0.47	0	2,2,2	0.61	0
5	EDO	A	203	-	3,3,3	0.75	0	2,2,2	0.48	0
5	EDO	E	204	-	3,3,3	0.38	0	2,2,2	0.33	0
5	EDO	E	202	-	3,3,3	0.35	0	2,2,2	0.56	0
5	EDO	B	201	-	3,3,3	0.58	0	2,2,2	0.38	0
5	EDO	A	204	-	3,3,3	0.36	0	2,2,2	0.61	0
5	EDO	B	206	-	3,3,3	0.48	0	2,2,2	0.44	0
5	EDO	D	203	-	3,3,3	0.55	0	2,2,2	0.30	0
5	EDO	F	101	-	3,3,3	0.42	0	2,2,2	1.21	0
6	GOL	A	207	-	5,5,5	1.11	0	5,5,5	0.86	0
5	EDO	A	205	-	3,3,3	0.42	0	2,2,2	0.90	0
4	EPE	D	201	-	15,15,15	1.11	1 (6%)	19,20,20	2.14	6 (31%)
5	EDO	D	206	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	E	205	-	3,3,3	0.36	0	2,2,2	0.58	0
5	EDO	A	202	-	3,3,3	0.24	0	2,2,2	0.78	0
5	EDO	F	102	-	3,3,3	0.47	0	2,2,2	0.37	0
6	GOL	A	208	-	5,5,5	0.99	1 (20%)	5,5,5	1.33	1 (20%)
5	EDO	F	103	-	3,3,3	0.37	0	2,2,2	0.73	0
5	EDO	D	207	-	3,3,3	0.74	0	2,2,2	0.12	0
6	GOL	B	209	-	5,5,5	1.27	1 (20%)	5,5,5	1.04	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
6	GOL	E	208	-	-	0/4/4/4	-
5	EDO	B	202	-	-	0/1/1/1	-
5	EDO	B	203	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	203	-	-	1/1/1/1	-
5	EDO	D	202	-	-	0/1/1/1	-
5	EDO	C	102	-	-	0/1/1/1	-
6	GOL	B	210	-	-	0/4/4/4	-
5	EDO	C	101	-	-	1/1/1/1	-
6	GOL	B	211	-	-	2/4/4/4	-
5	EDO	E	201	-	-	0/1/1/1	-
6	GOL	B	207	-	-	1/4/4/4	-
5	EDO	A	206	-	-	0/1/1/1	-
5	EDO	D	204	-	-	0/1/1/1	-
5	EDO	B	204	-	-	0/1/1/1	-
6	GOL	C	103	-	-	0/4/4/4	-
6	GOL	B	208	-	-	0/4/4/4	-
6	GOL	E	206	-	-	0/4/4/4	-
4	EPE	A	201	-	-	5/9/19/19	0/1/1/1
6	GOL	E	207	-	-	0/4/4/4	-
5	EDO	D	205	-	-	1/1/1/1	-
5	EDO	B	205	-	-	0/1/1/1	-
5	EDO	A	203	-	-	1/1/1/1	-
5	EDO	E	204	-	-	0/1/1/1	-
5	EDO	E	202	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
5	EDO	A	204	-	-	1/1/1/1	-
5	EDO	B	206	-	-	0/1/1/1	-
5	EDO	D	203	-	-	1/1/1/1	-
5	EDO	F	101	-	-	1/1/1/1	-
6	GOL	A	207	-	-	2/4/4/4	-
5	EDO	A	205	-	-	1/1/1/1	-
4	EPE	D	201	-	-	3/9/19/19	0/1/1/1
5	EDO	D	206	-	-	0/1/1/1	-
5	EDO	E	205	-	-	0/1/1/1	-
5	EDO	A	202	-	-	0/1/1/1	-
5	EDO	F	102	-	-	1/1/1/1	-
6	GOL	A	208	-	-	3/4/4/4	-
5	EDO	F	103	-	-	1/1/1/1	-
5	EDO	D	207	-	-	0/1/1/1	-
6	GOL	B	209	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	103	GOL	C1-C2	4.15	1.67	1.51
6	C	103	GOL	C3-C2	4.02	1.67	1.51
4	D	201	EPE	C10-S	3.67	1.82	1.77
6	B	207	GOL	C3-C2	3.42	1.64	1.51
4	A	201	EPE	C10-S	2.46	1.81	1.77
6	B	210	GOL	C3-C2	2.36	1.60	1.51
6	C	103	GOL	O3-C3	2.33	1.52	1.42
6	B	209	GOL	C1-C2	2.14	1.59	1.51
6	E	208	GOL	O2-C2	-2.14	1.37	1.43
6	A	208	GOL	C3-C2	2.13	1.59	1.51
6	B	211	GOL	C1-C2	2.02	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	EPE	C5-N4-C3	5.53	120.76	108.84
4	A	201	EPE	O1S-S-C10	4.96	114.22	106.73
4	A	201	EPE	C5-N4-C3	3.76	116.94	108.84
4	D	201	EPE	C2-C3-N4	3.33	117.37	110.65
4	D	201	EPE	C7-N4-C3	3.04	119.35	111.24
4	A	201	EPE	C7-N4-C5	2.97	119.15	111.24
4	D	201	EPE	C7-N4-C5	2.95	119.11	111.24
4	A	201	EPE	O2S-S-C10	2.92	111.14	106.73
4	D	201	EPE	C6-N1-C2	2.84	114.95	108.84
4	A	201	EPE	C7-N4-C3	2.32	117.42	111.24
4	D	201	EPE	O1S-S-C10	2.29	110.19	106.73
4	A	201	EPE	C2-C3-N4	2.27	115.23	110.65
6	A	208	GOL	O2-C2-C3	2.02	117.55	109.18

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	EPE	C10-C9-N1-C2
4	A	201	EPE	C10-C9-N1-C6
4	D	201	EPE	C10-C9-N1-C2
6	B	209	GOL	O1-C1-C2-C3
4	D	201	EPE	C8-C7-N4-C3
6	B	211	GOL	O1-C1-C2-O2
4	D	201	EPE	N4-C7-C8-O8
6	A	207	GOL	O1-C1-C2-C3
6	A	208	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	208	GOL	C1-C2-C3-O3
6	B	207	GOL	C1-C2-C3-O3
6	B	211	GOL	O1-C1-C2-C3
6	A	207	GOL	O1-C1-C2-O2
6	A	208	GOL	O1-C1-C2-O2
5	B	203	EDO	O1-C1-C2-O2
5	F	102	EDO	O1-C1-C2-O2
6	B	209	GOL	O1-C1-C2-O2
5	D	203	EDO	O1-C1-C2-O2
6	B	209	GOL	O2-C2-C3-O3
4	A	201	EPE	C9-C10-S-O2S
5	A	203	EDO	O1-C1-C2-O2
5	E	203	EDO	O1-C1-C2-O2
5	F	103	EDO	O1-C1-C2-O2
5	F	101	EDO	O1-C1-C2-O2
5	A	204	EDO	O1-C1-C2-O2
5	A	205	EDO	O1-C1-C2-O2
5	D	205	EDO	O1-C1-C2-O2
5	C	101	EDO	O1-C1-C2-O2
4	A	201	EPE	C9-C10-S-O3S
4	A	201	EPE	C8-C7-N4-C5

There are no ring outliers.

21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	208	GOL	5	0
5	B	202	EDO	2	0
5	E	203	EDO	1	0
5	D	202	EDO	6	0
5	C	102	EDO	1	0
6	B	211	GOL	1	0
5	A	206	EDO	1	0
6	B	208	GOL	1	0
5	D	205	EDO	1	0
5	B	205	EDO	1	0
5	A	203	EDO	1	0
5	A	204	EDO	2	0
5	B	206	EDO	3	0
6	A	207	GOL	1	0
5	A	205	EDO	1	0
4	D	201	EPE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	202	EDO	1	0
5	F	102	EDO	1	0
6	A	208	GOL	1	0
5	D	207	EDO	1	0
6	B	209	GOL	1	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	179/186 (96%)	-0.23	3 (1%) 69 73	10, 24, 48, 79	6 (3%)
1	D	179/186 (96%)	-0.20	2 (1%) 78 81	11, 25, 52, 76	2 (1%)
2	B	193/194 (99%)	0.04	8 (4%) 41 45	13, 29, 55, 74	1 (0%)
2	E	194/194 (100%)	0.05	9 (4%) 37 41	18, 29, 58, 81	0
3	C	13/13 (100%)	0.06	0 100 100	23, 29, 43, 60	0
3	F	13/13 (100%)	0.05	0 100 100	25, 30, 45, 49	0
All	All	771/786 (98%)	-0.08	22 (2%) 53 58	10, 27, 54, 81	9 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	106	THR	4.7
2	E	164	VAL	3.6
2	B	109	LEU	3.6
2	E	106	THR	3.5
2	B	139	LYS	3.4
2	E	-3	MET	3.1
1	A	129	THR	3.0
1	D	129	THR	3.0
1	D	130	THR	2.9
2	E	109	LEU	2.7
2	E	66	ASP	2.7
1	A	3	GLU	2.6
2	E	167	SER	2.6
2	B	108	PRO	2.6
2	B	188	TRP	2.4
2	E	165	PRO	2.4
2	B	111	HIS	2.3
2	B	165	PRO	2.3
2	B	190	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	111	HIS	2.3
1	A	181	ASP	2.1
2	E	112	HIS	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 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
6	GOL	B	211	6/6	0.70	0.19	59,64,69,69	0
6	GOL	B	207	6/6	0.74	0.18	44,56,61,67	0
5	EDO	B	205	4/4	0.74	0.14	51,53,54,61	0
5	EDO	A	204	4/4	0.77	0.16	49,55,63,68	0
5	EDO	C	102	4/4	0.79	0.17	41,50,51,62	0
6	GOL	A	207	6/6	0.79	0.17	53,55,63,66	0
5	EDO	F	103	4/4	0.80	0.15	49,52,54,59	0
5	EDO	D	205	4/4	0.81	0.18	51,55,55,62	0
5	EDO	A	202	4/4	0.82	0.19	52,52,53,53	0
5	EDO	F	101	4/4	0.83	0.17	37,40,57,58	0
5	EDO	A	206	4/4	0.84	0.12	46,49,57,62	0
5	EDO	B	206	4/4	0.84	0.14	50,52,53,57	0
5	EDO	B	202	4/4	0.84	0.14	36,40,46,49	0
5	EDO	E	205	4/4	0.85	0.15	46,50,53,58	0
6	GOL	B	208	6/6	0.85	0.13	41,45,52,60	0
5	EDO	D	207	4/4	0.85	0.18	35,41,54,60	0
4	EPE	D	201	15/15	0.86	0.14	45,56,66,71	0
5	EDO	D	203	4/4	0.86	0.15	37,47,48,56	0
5	EDO	F	102	4/4	0.86	0.12	46,52,52,57	0
5	EDO	E	203	4/4	0.86	0.12	40,42,43,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	E	208	6/6	0.86	0.12	34,45,53,66	0
5	EDO	E	204	4/4	0.87	0.11	43,49,57,58	0
5	EDO	A	205	4/4	0.87	0.13	44,45,52,55	0
5	EDO	C	101	4/4	0.87	0.17	34,46,55,57	0
4	EPE	A	201	15/15	0.87	0.15	37,48,72,75	0
5	EDO	D	202	4/4	0.87	0.22	34,39,43,49	0
5	EDO	E	202	4/4	0.88	0.13	34,47,54,63	0
6	GOL	C	103	6/6	0.89	0.12	30,37,45,47	0
5	EDO	A	203	4/4	0.89	0.15	32,36,36,46	0
6	GOL	E	207	6/6	0.90	0.13	31,48,54,54	0
5	EDO	B	204	4/4	0.90	0.12	41,43,45,47	0
5	EDO	D	204	4/4	0.91	0.13	40,44,49,53	0
6	GOL	A	208	6/6	0.91	0.10	39,39,45,55	0
6	GOL	E	206	6/6	0.91	0.10	29,46,48,50	0
6	GOL	B	209	6/6	0.91	0.12	27,41,49,53	0
6	GOL	B	210	6/6	0.91	0.10	30,39,49,50	0
5	EDO	D	206	4/4	0.92	0.14	27,43,51,65	0
5	EDO	B	203	4/4	0.92	0.11	34,40,40,40	0
5	EDO	E	201	4/4	0.96	0.08	28,31,31,32	0
5	EDO	B	201	4/4	0.97	0.07	25,29,29,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.