Full wwPDB X-ray Structure Validation Report (i)

May 1, 2016 – 07:28 AM EDT

PDB ID	:	5EU6
Title	:	HLA Class I antigen
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Deposited on	:	2015-11-18
Resolution	:	2.02 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:

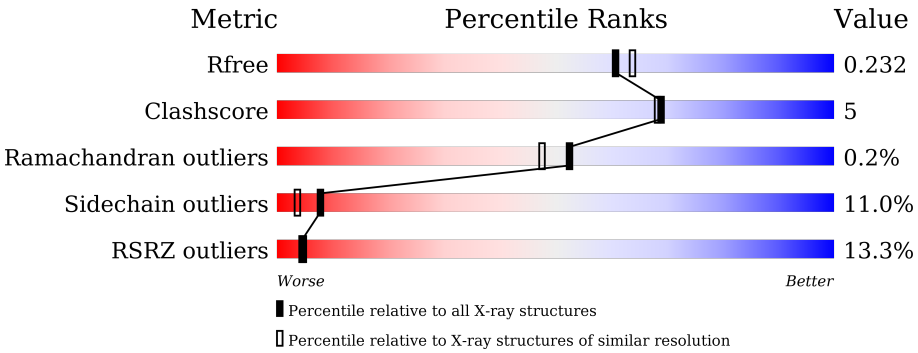
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.02 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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	276	7% 81% 15% ·
2	B	100	4% 81% 18% ·
3	C	9	89% 11%
4	D	204	28% 73% 22% 5%
5	E	244	13% 84% 12% ·

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
6	EDO	A	301	-	-	-	X
6	EDO	A	302	-	-	-	X
6	EDO	A	306	-	-	-	X
6	EDO	D	301	-	-	-	X
6	EDO	E	301	-	-	-	X
7	GOL	A	307	-	-	-	X
7	GOL	D	303	-	-	-	X
7	GOL	E	302	-	-	-	X
8	SO4	A	309	-	-	-	X
8	SO4	A	311	-	-	-	X
8	SO4	B	302	-	-	-	X
8	SO4	B	304	-	-	-	X
8	SO4	E	303	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6980 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 I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2261	1412	411	429	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called TYR-LEU-GLU-PRO-GLY-PRO-VAL-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			69	46	9	14			

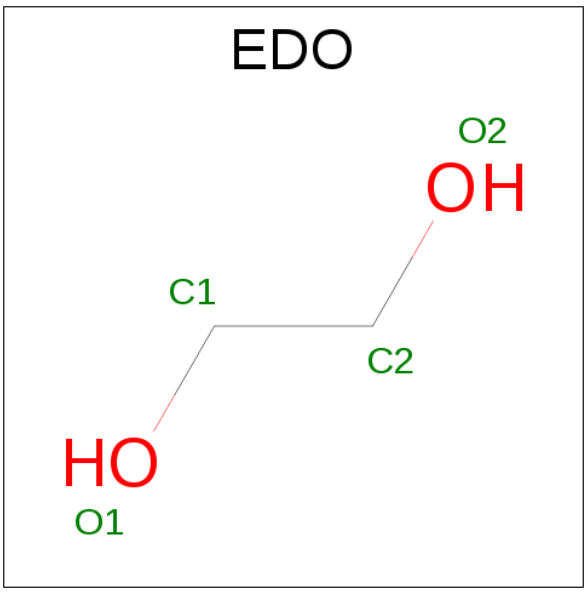
- Molecule 4 is a protein called Human TCR Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	204	Total	C	N	O	S	0	0	0
			1559	967	261	323	8			

- Molecule 5 is a protein called Human TCR Heavy Chain.

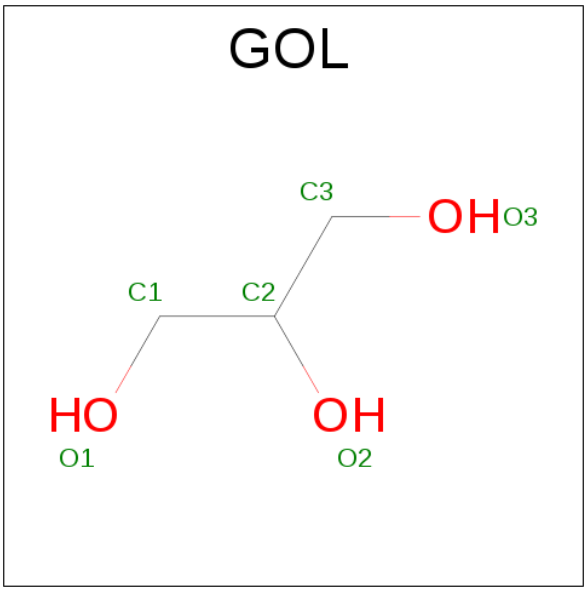
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	244	Total	C	N	O	S	0	1	0
			1923	1211	333	373	6			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



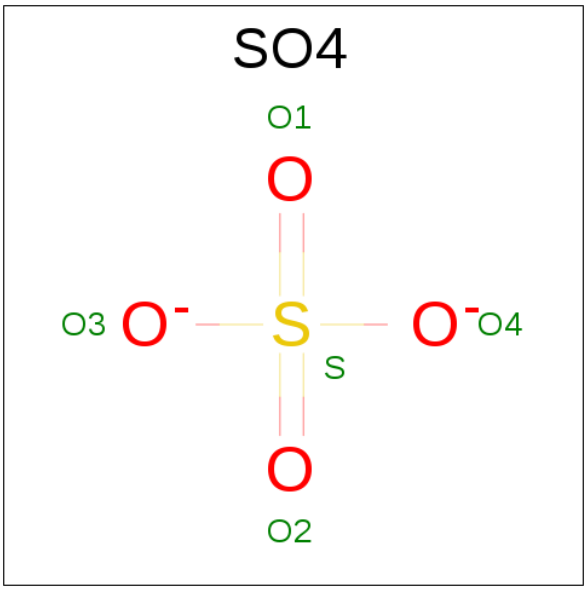
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	E	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

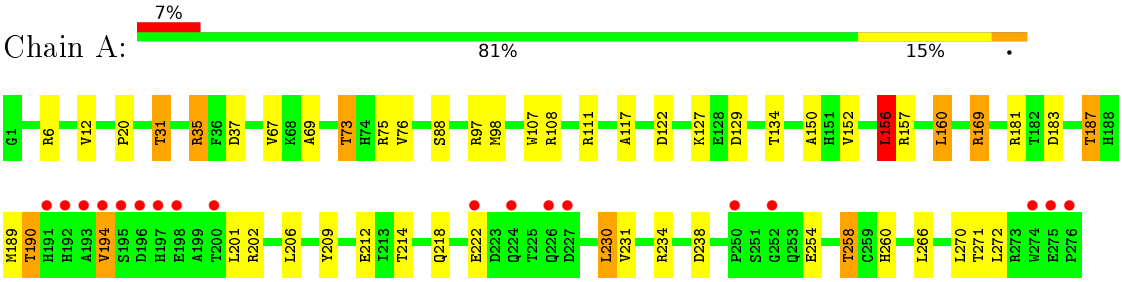
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	98	Total O 98 98	0	0
9	B	27	Total O 27 27	0	0
9	C	4	Total O 4 4	0	0
9	D	52	Total O 52 52	0	0
9	E	52	Total O 52 52	0	0

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.

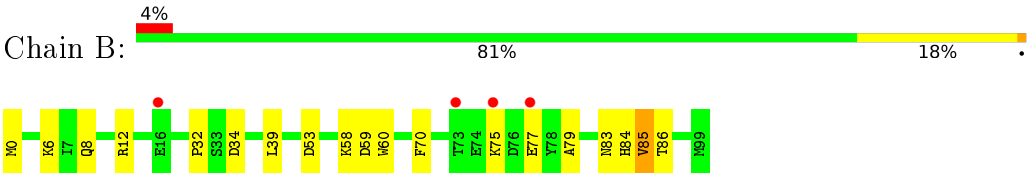
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain A:



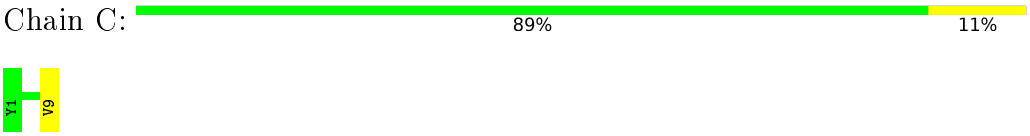
- Molecule 2: Beta-2-microglobulin

Chain B:



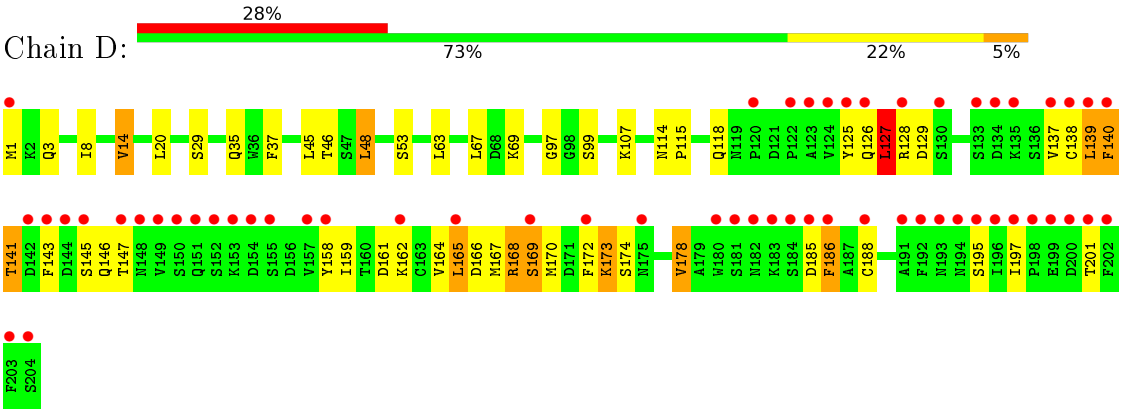
- Molecule 3: TYR-LEU-GLU-PRO-GLY-PRO-VAL-THR-VAL

Chain C:



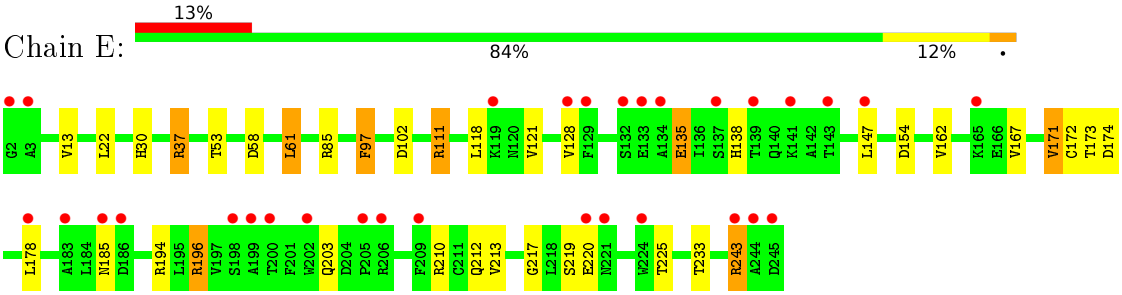
- Molecule 4: Human TCR Light Chain

Chain D:



- Molecule 5: Human TCR Heavy Chain

Chain E:


13%
84%
12%
G2
A3
V13
L22
H30
R37
T53
D58
L61
R85
F97
D102
R111
L118
K119
N120
V121
V128
F129
S132
E133
A134
E135
I136
S137
H138
T139
Q140
K141
A142
T143
L147
D154
V162
K165
E166
V167
V171
C172
T173
D174
L178
A183
L184
N185
D186
R194
L195
R196
V197
S198
A199
T200
F201
W202
Q203
D204
P205
R206
F209
R210
C211
Q212
V213
G217
L218
S219
E220
W221
W224
T225
T233
R243
A244
D245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	45.52Å 54.41Å 112.12Å 85.01° 81.64° 72.63°	Depositor
Resolution (Å)	51.87 – 2.02 51.87 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.7 (51.87-2.02) 96.2 (51.87-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.222 0.198 , 0.232	Depositor DCC
R_{free} test set	3294 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6980	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	0.98	0/2327	1.15	18/3159 (0.6%)
2	B	0.97	2/860 (0.2%)	1.03	5/1162 (0.4%)
3	C	1.09	1/71 (1.4%)	1.00	0/97
4	D	0.94	0/1586	0.98	4/2149 (0.2%)
5	E	0.79	0/1975	0.97	6/2688 (0.2%)
All	All	0.92	3/6819 (0.0%)	1.04	33/9255 (0.4%)

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	A	0	1
4	D	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	77	GLU	CG-CD	6.64	1.61	1.51
3	C	9	VAL	C-OXT	5.24	1.33	1.23
2	B	77	GLU	CD-OE2	5.10	1.31	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	37	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	A	108	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	37	ASP	CB-CG-OD1	9.80	127.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH2	7.90	124.25	120.30
5	E	111	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	160	LEU	CB-CG-CD1	7.55	123.84	111.00
2	B	34	ASP	CB-CG-OD1	7.45	125.01	118.30
2	B	85	VAL	CB-CA-C	-6.87	98.35	111.40
1	A	157	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	6	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	75	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	111	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	97	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	129	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	169	ARG	NE-CZ-NH1	6.17	123.39	120.30
5	E	37	ARG	NE-CZ-NH2	6.04	123.32	120.30
4	D	107	LYS	CD-CE-NZ	-6.02	97.86	111.70
5	E	102	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	122	ASP	CB-CG-OD1	5.82	123.53	118.30
4	D	127	LEU	CA-CB-CG	5.62	128.21	115.30
5	E	174	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	111	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	238	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	B	53	ASP	CB-CG-OD2	5.45	123.21	118.30
2	B	77	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	156	LEU	CB-CG-CD1	5.40	120.19	111.00
1	A	35	ARG	NE-CZ-NH1	5.39	123.00	120.30
4	D	48	LEU	CB-CG-CD1	5.34	120.08	111.00
4	D	48	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	6	ARG	NE-CZ-NH2	5.25	122.93	120.30
2	B	59	ASP	CB-CG-OD1	5.19	122.97	118.30
5	E	97	PHE	CB-CG-CD1	5.05	124.33	120.80
1	A	169	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	VAL	Peptide
4	D	1	MET	Peptide
4	D	174	SER	Peptide
4	D	186	PHE	Peptide

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	2261	0	2109	22	0
2	B	837	0	803	5	0
3	C	69	0	70	0	0
4	D	1559	0	1506	27	0
5	E	1923	0	1820	15	0
6	A	24	0	35	2	0
6	B	4	0	6	1	0
6	D	8	0	12	0	0
6	E	4	0	6	2	0
7	A	6	0	8	1	0
7	D	6	0	8	3	0
7	E	6	0	8	0	0
8	A	20	0	0	0	0
8	B	15	0	0	0	0
8	E	5	0	0	0	0
9	A	98	0	0	1	0
9	B	27	0	0	0	0
9	C	4	0	0	0	0
9	D	52	0	0	0	0
9	E	52	0	0	0	0
All	All	6980	0	6391	61	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 (61) 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)
4:D:14:VAL:HG11	4:D:20:LEU:HD21	1.60	0.81
4:D:3:GLN:HB2	7:D:303:GOL:H2	1.66	0.77
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.73	0.71
1:A:69:ALA:O	1:A:73:THR:HG23	1.91	0.70
4:D:165:LEU:HB2	5:E:172:CYS:HB3	1.75	0.69
5:E:217:GLY:H	5:E:233:THR:HG22	1.58	0.67
4:D:127:LEU:HD21	4:D:137:VAL:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE2	1:A:134[B]:THR:HG23	1.80	0.63
4:D:3:GLN:CB	7:D:303:GOL:H2	2.28	0.61
1:A:187:THR:CG2	1:A:272:LEU:HD11	2.31	0.61
7:A:307:GOL:H32	4:D:99:SER:HB2	1.83	0.60
5:E:210:ARG:NH2	5:E:212:GLN:OE1	2.34	0.60
1:A:212:GLU:HG2	9:A:405:HOH:O	2.02	0.60
2:B:84:HIS:HD2	2:B:86:THR:OG1	1.86	0.58
4:D:141:THR:HG23	4:D:173:LYS:HG2	1.86	0.57
1:A:150:ALA:O	6:A:306:EDO:H22	2.04	0.56
5:E:118:LEU:O	5:E:121:VAL:HG13	2.05	0.56
4:D:143:PHE:CZ	4:D:173:LYS:HE2	2.42	0.55
1:A:218:GLN:HB2	1:A:258:THR:HG23	1.90	0.54
4:D:165:LEU:HG	5:E:171:VAL:O	2.07	0.54
1:A:152:VAL:HG12	1:A:156:LEU:HD22	1.91	0.53
5:E:217:GLY:N	5:E:233:THR:HG22	2.23	0.53
5:E:53:THR:HG23	6:E:301:EDO:H21	1.91	0.53
4:D:127:LEU:HD21	4:D:137:VAL:CG2	2.38	0.52
5:E:58:ASP:HB2	5:E:61:LEU:HD22	1.89	0.52
4:D:129:ASP:HB3	5:E:128:VAL:O	2.10	0.52
1:A:260:HIS:CE1	1:A:271:THR:HG23	2.45	0.52
1:A:20:PRO:HD3	6:A:305:EDO:H21	1.90	0.52
4:D:165:LEU:HD13	4:D:166:ASP:H	1.75	0.52
4:D:167:MET:SD	5:E:196:ARG:HG2	2.50	0.52
1:A:187:THR:HG23	1:A:272:LEU:HD21	1.92	0.50
4:D:114:ASN:HB3	4:D:143:PHE:CZ	2.47	0.50
4:D:197:ILE:HG21	5:E:138:HIS:CE1	2.47	0.49
4:D:97:GLY:HA3	7:D:303:GOL:H31	1.93	0.49
4:D:158:TYR:HB2	4:D:178:VAL:HG13	1.93	0.49
4:D:173:LYS:HE3	4:D:173:LYS:HA	1.94	0.49
1:A:234:ARG:HH21	2:B:8:GLN:NE2	2.12	0.48
1:A:189:MET:CE	1:A:201:LEU:HD23	2.44	0.47
5:E:111:ARG:NH2	5:E:154:ASP:OD1	2.39	0.47
4:D:29:SER:HB2	4:D:69:LYS:O	2.14	0.47
4:D:115:PRO:HG2	4:D:164:VAL:HG21	1.97	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.45
1:A:190:THR:CG2	1:A:202:ARG:HB3	2.44	0.45
4:D:114:ASN:HB3	4:D:143:PHE:CE2	2.52	0.45
4:D:139:LEU:HG	4:D:140:PHE:N	2.33	0.43
4:D:126:GLN:NE2	4:D:185:ASP:OD2	2.52	0.43
2:B:32:PRO:O	2:B:84:HIS:HE1	2.01	0.43
4:D:53:SER:HB2	4:D:69:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:CE	1:A:134[B]:THR:HG23	2.48	0.42
4:D:125:TYR:CZ	5:E:135:GLU:HB2	2.54	0.42
1:A:31:THR:CG2	1:A:209:TYR:OH	2.68	0.42
1:A:230:LEU:HD12	1:A:230:LEU:H	1.84	0.42
1:A:201:LEU:HD11	1:A:254:GLU:HG3	2.01	0.41
4:D:165:LEU:O	4:D:172:PHE:CD1	2.73	0.41
2:B:79:ALA:HB2	6:B:301:EDO:H21	2.01	0.41
1:A:76:VAL:HG22	6:E:301:EDO:H12	2.02	0.41
5:E:162:VAL:HG12	5:E:167:VAL:CG2	2.51	0.41
1:A:107:TRP:HB3	1:A:169:ARG:HD3	2.03	0.41
5:E:203:GLN:HA	5:E:243:ARG:O	2.21	0.41
1:A:181:ARG:NH2	1:A:183:ASP:OD2	2.47	0.40
4:D:35:GLN:HG3	4:D:37:PHE:CE2	2.56	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	275/276 (100%)	269 (98%)	6 (2%)	0	100 100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100 100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
4	D	202/204 (99%)	183 (91%)	17 (8%)	2 (1%)	19 10
5	E	243/244 (100%)	237 (98%)	6 (2%)	0	100 100
All	All	825/833 (99%)	791 (96%)	32 (4%)	2 (0%)	52 47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	168	ARG

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Mol	Chain	Res	Type
4	D	169	SER

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	233/232 (100%)	213 (91%)	20 (9%)	13 7
2	B	95/95 (100%)	86 (90%)	9 (10%)	11 5
3	C	8/8 (100%)	8 (100%)	0	100 100
4	D	180/180 (100%)	150 (83%)	30 (17%)	3 1
5	E	207/206 (100%)	187 (90%)	20 (10%)	10 5
All	All	723/721 (100%)	644 (89%)	79 (11%)	8 4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	31	THR
1	A	35	ARG
1	A	67	VAL
1	A	73	THR
1	A	88	SER
1	A	98	MET
1	A	156	LEU
1	A	160	LEU
1	A	187	THR
1	A	190	THR
1	A	194	VAL
1	A	206	LEU
1	A	214	THR
1	A	222	GLU
1	A	230	LEU
1	A	231	VAL
1	A	258	THR

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Mol	Chain	Res	Type
1	A	266	LEU
1	A	270	LEU
2	B	0	MET
2	B	6	LYS
2	B	12	ARG
2	B	39	LEU
2	B	58	LYS
2	B	70	PHE
2	B	75	LYS
2	B	83	ASN
2	B	85	VAL
4	D	8	ILE
4	D	14	VAL
4	D	45	LEU
4	D	46	THR
4	D	48	LEU
4	D	63	LEU
4	D	67	LEU
4	D	118	GLN
4	D	127	LEU
4	D	128	ARG
4	D	138	CYS
4	D	139	LEU
4	D	140	PHE
4	D	141	THR
4	D	145	SER
4	D	146	GLN
4	D	147	THR
4	D	159	ILE
4	D	161	ASP
4	D	162	LYS
4	D	165	LEU
4	D	168	ARG
4	D	169	SER
4	D	170	MET
4	D	173	LYS
4	D	178	VAL
4	D	186	PHE
4	D	188	CYS
4	D	195	SER
4	D	201	THR
5	E	13	VAL

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Mol	Chain	Res	Type
5	E	22	LEU
5	E	30	HIS
5	E	37	ARG
5	E	61	LEU
5	E	85	ARG
5	E	97	PHE
5	E	135	GLU
5	E	147	LEU
5	E	171	VAL
5	E	173	THR
5	E	178	LEU
5	E	185	ASN
5	E	194	ARG
5	E	196	ARG
5	E	213	VAL
5	E	219	SER
5	E	220	GLU
5	E	225	THR
5	E	243	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	70	HIS
1	A	262	GLN
2	B	8	GLN
2	B	51	HIS
2	B	83	ASN
2	B	84	HIS
4	D	64	ASN
4	D	82	GLN
5	E	30	HIS
5	E	138	HIS
5	E	140	GLN
5	E	234	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

21 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	EDO	A	301	-	3,3,3	0.45	0	2,2,2	0.45	0
6	EDO	A	302	-	3,3,3	0.33	0	2,2,2	0.79	0
6	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.23	0
6	EDO	A	304	-	3,3,3	0.52	0	2,2,2	0.49	0
6	EDO	A	305	-	3,3,3	0.84	0	2,2,2	0.80	0
6	EDO	A	306	-	3,3,3	0.55	0	2,2,2	0.06	0
7	GOL	A	307	-	5,5,5	0.27	0	5,5,5	0.48	0
8	SO4	A	308	-	4,4,4	0.45	0	6,6,6	0.32	0
8	SO4	A	309	-	4,4,4	0.67	0	6,6,6	0.49	0
8	SO4	A	310	-	4,4,4	0.59	0	6,6,6	0.43	0
8	SO4	A	311	-	4,4,4	0.50	0	6,6,6	0.34	0
6	EDO	B	301	-	3,3,3	0.21	0	2,2,2	0.68	0
8	SO4	B	302	-	4,4,4	0.69	0	6,6,6	0.23	0
8	SO4	B	303	-	4,4,4	0.46	0	6,6,6	0.19	0
8	SO4	B	304	-	4,4,4	0.35	0	6,6,6	0.36	0
6	EDO	D	301	-	3,3,3	0.36	0	2,2,2	0.54	0
6	EDO	D	302	-	3,3,3	0.40	0	2,2,2	0.50	0
7	GOL	D	303	-	5,5,5	0.34	0	5,5,5	0.85	0
6	EDO	E	301	-	3,3,3	0.52	0	2,2,2	0.26	0
7	GOL	E	302	-	5,5,5	0.47	0	5,5,5	0.48	0
8	SO4	E	303	-	4,4,4	0.51	0	6,6,6	0.39	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	EDO	A	301	-	-	0/1/1/1	0/0/0/0
6	EDO	A	302	-	-	0/1/1/1	0/0/0/0
6	EDO	A	303	-	-	0/1/1/1	0/0/0/0
6	EDO	A	304	-	-	0/1/1/1	0/0/0/0
6	EDO	A	305	-	-	0/1/1/1	0/0/0/0
6	EDO	A	306	-	-	0/1/1/1	0/0/0/0
7	GOL	A	307	-	-	0/4/4/4	0/0/0/0
8	SO4	A	308	-	-	0/0/0/0	0/0/0/0
8	SO4	A	309	-	-	0/0/0/0	0/0/0/0
8	SO4	A	310	-	-	0/0/0/0	0/0/0/0
8	SO4	A	311	-	-	0/0/0/0	0/0/0/0
6	EDO	B	301	-	-	0/1/1/1	0/0/0/0
8	SO4	B	302	-	-	0/0/0/0	0/0/0/0
8	SO4	B	303	-	-	0/0/0/0	0/0/0/0
8	SO4	B	304	-	-	0/0/0/0	0/0/0/0
6	EDO	D	301	-	-	0/1/1/1	0/0/0/0
6	EDO	D	302	-	-	0/1/1/1	0/0/0/0
7	GOL	D	303	-	-	0/4/4/4	0/0/0/0
6	EDO	E	301	-	-	0/1/1/1	0/0/0/0
7	GOL	E	302	-	-	0/4/4/4	0/0/0/0
8	SO4	E	303	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	EDO	1	0
6	A	306	EDO	1	0
7	A	307	GOL	1	0
6	B	301	EDO	1	0
7	D	303	GOL	3	0
6	E	301	EDO	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, 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	276/276 (100%)	0.49	18 (6%) 22 23	22, 39, 102, 142	0
2	B	100/100 (100%)	0.21	4 (4%) 42 44	26, 45, 70, 80	0
3	C	9/9 (100%)	0.15	0 100 100	25, 26, 31, 33	0
4	D	204/204 (100%)	1.73	58 (28%) 1 1	23, 47, 130, 160	0
5	E	244/244 (100%)	0.62	31 (12%) 5 5	24, 58, 99, 125	0
All	All	833/833 (100%)	0.79	111 (13%) 4 5	22, 46, 115, 160	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	198	PRO	15.6
4	D	202	PHE	12.4
4	D	201	THR	11.6
4	D	155	SER	10.2
4	D	203	PHE	10.0
4	D	200	ASP	10.0
4	D	195	SER	10.0
4	D	204	SER	9.8
4	D	123	ALA	9.5
4	D	154	ASP	9.0
4	D	196	ILE	8.9
4	D	194	ASN	8.5
1	A	276	PRO	8.4
4	D	199	GLU	8.2
4	D	192	PHE	7.8
4	D	153	LYS	7.6
4	D	152	SER	7.6
4	D	180	TRP	7.1
4	D	165	LEU	7.0
4	D	191	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
5	E	199	ALA	6.9
4	D	143	PHE	6.8
1	A	193	ALA	6.6
5	E	245	ASP	6.0
5	E	137	SER	5.4
4	D	133	SER	5.3
1	A	197	HIS	5.3
1	A	274	TRP	5.1
4	D	124	VAL	5.0
1	A	194	VAL	4.8
4	D	135	LYS	4.8
5	E	2	GLY	4.8
4	D	147	THR	4.6
1	A	195	SER	4.5
4	D	197	ILE	4.4
4	D	151	GLN	4.3
4	D	175	ASN	4.2
4	D	172	PHE	4.2
5	E	202	TRP	4.2
5	E	139	THR	4.1
4	D	182	ASN	4.1
4	D	140	PHE	4.1
4	D	138	CYS	4.0
5	E	221	ASN	4.0
4	D	134	ASP	4.0
5	E	3	ALA	3.9
4	D	186	PHE	3.9
5	E	209	PHE	3.8
4	D	150	SER	3.8
5	E	129	PHE	3.8
4	D	185	ASP	3.7
1	A	192	HIS	3.7
1	A	224	GLN	3.7
4	D	184	SER	3.7
4	D	149	VAL	3.7
5	E	134	ALA	3.5
4	D	183	LYS	3.4
4	D	128	ARG	3.3
1	A	275	GLU	3.3
4	D	137	VAL	3.3
4	D	120	PRO	3.3
5	E	206	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	220	GLU	3.2
4	D	148	ASN	3.2
4	D	193	ASN	3.2
1	A	200	THR	3.1
4	D	1	MET	3.1
5	E	133	GLU	3.1
4	D	188	CYS	3.0
2	B	73	THR	3.0
4	D	125	TYR	3.0
5	E	143	THR	2.9
1	A	227	ASP	2.9
2	B	75	LYS	2.9
5	E	200	THR	2.9
2	B	16	GLU	2.8
1	A	252	GLY	2.8
4	D	139	LEU	2.7
4	D	145	SER	2.7
5	E	244	ALA	2.7
4	D	157	VAL	2.6
5	E	185	ASN	2.6
5	E	205	PRO	2.6
1	A	198	GLU	2.6
5	E	147	LEU	2.6
1	A	196	ASP	2.6
1	A	222	GLU	2.6
4	D	142	ASP	2.6
5	E	224	TRP	2.6
5	E	243	ARG	2.5
4	D	181	SER	2.5
5	E	183	ALA	2.4
1	A	226	GLN	2.4
4	D	130	SER	2.4
4	D	126	GLN	2.4
1	A	191	HIS	2.3
5	E	165	LYS	2.3
4	D	122	PRO	2.3
5	E	198	SER	2.3
4	D	144	ASP	2.2
5	E	132	SER	2.2
2	B	77	GLU	2.2
1	A	250	PRO	2.2
5	E	178	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	162	LYS	2.2
5	E	128	VAL	2.1
5	E	186	ASP	2.1
5	E	119	LYS	2.1
4	D	169	SER	2.1
4	D	158	TYR	2.1
5	E	141	LYS	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 carbohydrates 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. 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
8	SO4	A	309	5/5	0.71	0.32	24.57	38,47,52,53	5
8	SO4	B	304	5/5	0.89	0.42	13.13	72,94,98,99	0
7	GOL	E	302	6/6	0.61	0.31	9.73	66,72,75,75	0
8	SO4	B	302	5/5	0.88	0.27	9.67	56,65,79,82	0
8	SO4	E	303	5/5	0.84	0.32	9.45	73,78,85,90	0
8	SO4	A	311	5/5	0.96	0.27	6.73	69,79,79,83	0
6	EDO	E	301	4/4	0.86	0.22	5.04	48,51,58,60	0
6	EDO	A	306	4/4	0.80	0.21	4.81	50,52,56,60	0
6	EDO	D	301	4/4	0.89	0.17	3.65	49,50,51,52	0
7	GOL	A	307	6/6	0.82	0.22	3.01	55,58,60,68	0
7	GOL	D	303	6/6	0.80	0.30	2.80	47,53,61,62	0
6	EDO	A	301	4/4	0.78	0.18	2.64	49,55,60,60	0
6	EDO	A	302	4/4	0.88	0.18	2.20	46,48,50,53	0
6	EDO	A	303	4/4	0.95	0.17	1.54	37,46,50,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	EDO	A	304	4/4	0.94	0.14	1.44	48,50,50,51	0
6	EDO	A	305	4/4	0.92	0.18	1.30	31,34,40,40	0
6	EDO	B	301	4/4	0.96	0.12	-0.60	33,36,36,46	0
6	EDO	D	302	4/4	0.94	0.12	-0.62	49,53,54,56	0
8	SO4	A	310	5/5	0.69	0.33	-	66,85,101,104	0
8	SO4	A	308	5/5	0.88	0.27	-	80,86,91,92	0
8	SO4	B	303	5/5	0.83	0.29	-	84,91,105,105	0

6.5 Other polymers

There are no such residues in this entry.