



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:33 PM GMT

PDB ID : 3U0P
Title : Crystal structure of human CD1d-lysophosphatidylcholine
Authors : Lopez-Sagaseta, J.; Sibener, L.V.; Adams, E.J.
Deposited on : 2011-09-28
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

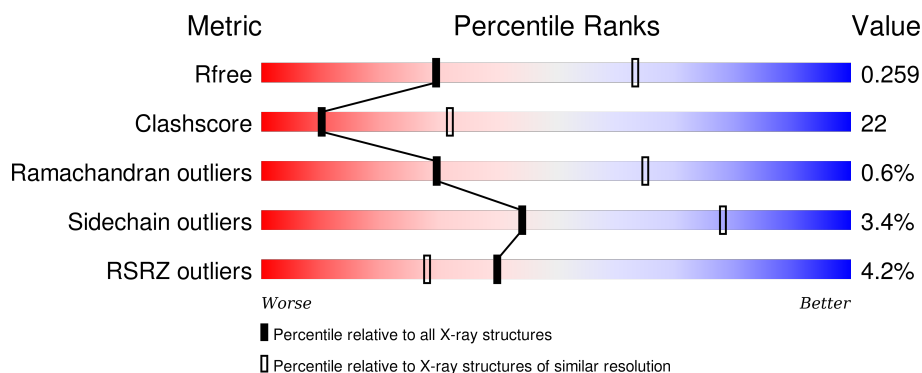
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 $\leq 5\%$. 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	284	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>
1	C	284	<div> <div>65%</div> <div>30%</div> <div>• •</div> </div>
1	E	284	<div> <div>4%</div> <div>55%</div> <div>23%</div> <div>•</div> <div>20%</div> </div>
2	B	102	<div> <div>%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
2	D	102	<div> <div>66%</div> <div>29%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	102	

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
11	NBU	E	303	-	-	-	X
4	LSC	A	305	-	-	-	X
4	LSC	C	304	-	-	-	X
5	HEX	A	306	-	-	-	X
6	SO4	A	307	-	-	X	-
6	SO4	C	306	-	-	-	X
6	SO4	C	309	-	-	-	X
7	GOL	A	310	-	-	-	X
7	GOL	B	3000	-	-	-	X
8	UND	A	312	-	-	-	X
9	NAG	C	301	-	-	X	-
9	FUC	C	303	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8983 atoms, of which 12 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	26	0	0
			2198	1406	385	400	7			
1	C	274	Total	C	N	O	S	57	0	0
			2208	1412	388	401	7			
1	E	228	Total	C	N	O	S	133	0	0
			1843	1187	314	337	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	EXPRESSION TAG	UNP P15813
A	1	ASP	-	EXPRESSION TAG	UNP P15813
A	2	PRO	-	EXPRESSION TAG	UNP P15813
A	42	GLN	ASN	ENGINEERED MUTATION	UNP P15813
A	108	GLN	ASN	ENGINEERED MUTATION	UNP P15813
A	163	GLN	ASN	ENGINEERED MUTATION	UNP P15813
A	278	HIS	-	EXPRESSION TAG	UNP P15813
A	279	HIS	-	EXPRESSION TAG	UNP P15813
A	280	HIS	-	EXPRESSION TAG	UNP P15813
A	281	HIS	-	EXPRESSION TAG	UNP P15813
A	282	HIS	-	EXPRESSION TAG	UNP P15813
A	283	HIS	-	EXPRESSION TAG	UNP P15813
C	0	ALA	-	EXPRESSION TAG	UNP P15813
C	1	ASP	-	EXPRESSION TAG	UNP P15813
C	2	PRO	-	EXPRESSION TAG	UNP P15813
C	42	GLN	ASN	ENGINEERED MUTATION	UNP P15813
C	108	GLN	ASN	ENGINEERED MUTATION	UNP P15813
C	163	GLN	ASN	ENGINEERED MUTATION	UNP P15813
C	278	HIS	-	EXPRESSION TAG	UNP P15813
C	279	HIS	-	EXPRESSION TAG	UNP P15813
C	280	HIS	-	EXPRESSION TAG	UNP P15813
C	281	HIS	-	EXPRESSION TAG	UNP P15813
C	282	HIS	-	EXPRESSION TAG	UNP P15813

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Chain	Residue	Modelled	Actual	Comment	Reference
C	283	HIS	-	EXPRESSION TAG	UNP P15813
E	0	ALA	-	EXPRESSION TAG	UNP P15813
E	1	ASP	-	EXPRESSION TAG	UNP P15813
E	2	PRO	-	EXPRESSION TAG	UNP P15813
E	42	GLN	ASN	ENGINEERED MUTATION	UNP P15813
E	108	GLN	ASN	ENGINEERED MUTATION	UNP P15813
E	163	GLN	ASN	ENGINEERED MUTATION	UNP P15813
E	278	HIS	-	EXPRESSION TAG	UNP P15813
E	279	HIS	-	EXPRESSION TAG	UNP P15813
E	280	HIS	-	EXPRESSION TAG	UNP P15813
E	281	HIS	-	EXPRESSION TAG	UNP P15813
E	282	HIS	-	EXPRESSION TAG	UNP P15813
E	283	HIS	-	EXPRESSION TAG	UNP P15813

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	9	0	0
			828	528	140	157	3			
2	D	100	Total	C	N	O	S	14	0	0
			835	533	141	158	3			
2	F	82	Total	C	N	O	S	12	0	0
			636	410	108	116	2			

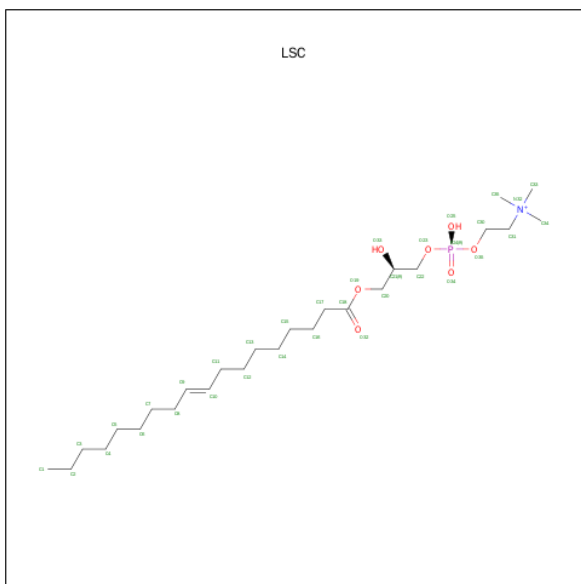
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	EXPRESSION TAG	UNP P61769
B	-1	ASP	-	EXPRESSION TAG	UNP P61769
B	0	PRO	-	EXPRESSION TAG	UNP P61769
D	-2	ALA	-	EXPRESSION TAG	UNP P61769
D	-1	ASP	-	EXPRESSION TAG	UNP P61769
D	0	PRO	-	EXPRESSION TAG	UNP P61769
F	-2	ALA	-	EXPRESSION TAG	UNP P61769
F	-1	ASP	-	EXPRESSION TAG	UNP P61769
F	0	PRO	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

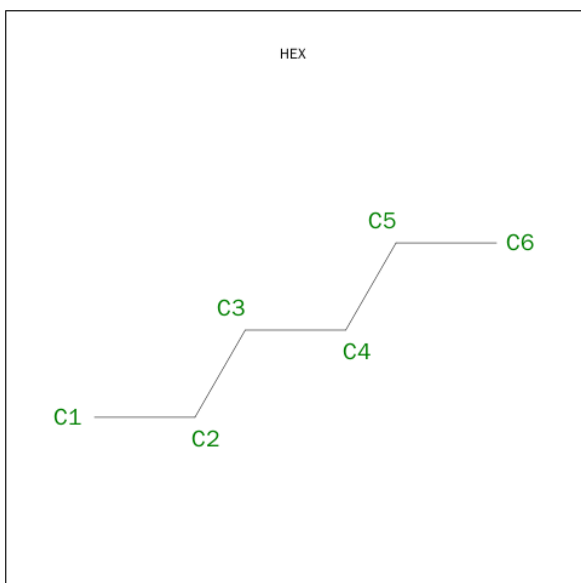
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			48	28	2	18		

- Molecule 4 is (4R,7R,18E)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-18-EN-1-AMINIUM 4-OXIDE (three-letter code: LSC) (formula: $C_{26}H_{53}NO_7P$).



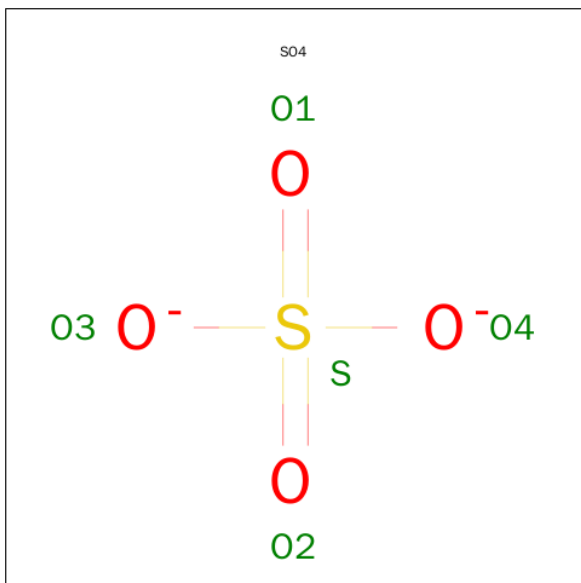
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			35	26	1	7	1		
4	C	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

- Molecule 5 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



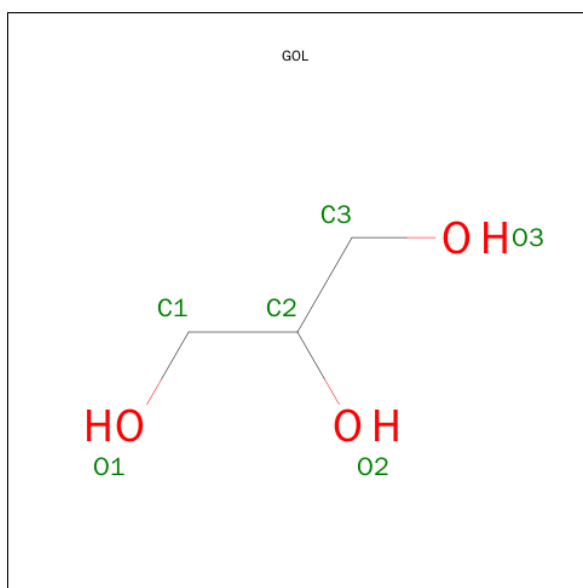
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 6 6	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



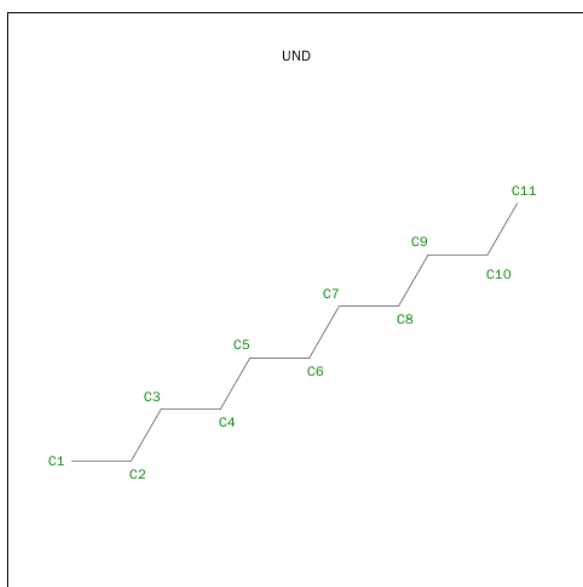
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0

- 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	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 11 11	0	0

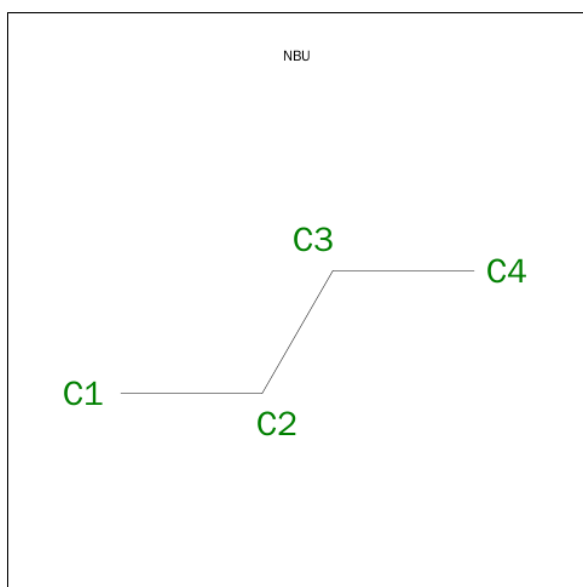
- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total C N O 34 20 1 13	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	2	Total C N O 24 14 1 9	0	0

- Molecule 11 is N-BUTANE (three-letter code: NBU) (formula: C₄H₁₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	1	Total C 4 4	0	0

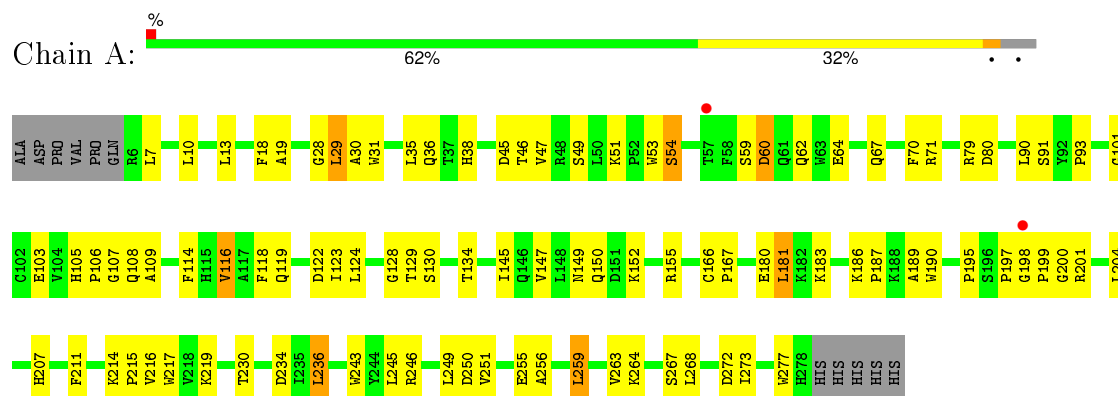
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	58	Total H O 68 10 58	0	0
12	B	20	Total O 20 20	0	0
12	C	31	Total O 31 31	0	0
12	D	10	Total H O 12 2 10	0	0
12	E	8	Total O 8 8	0	0
12	F	2	Total O 2 2	0	0

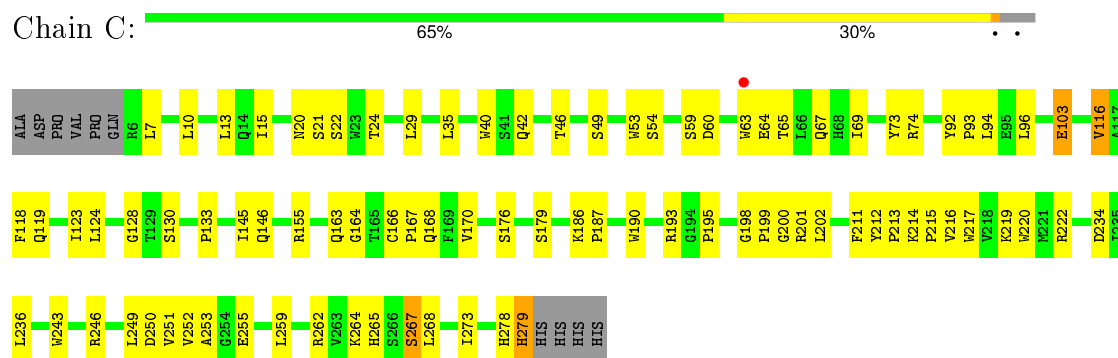
3 Residue-property plots

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.

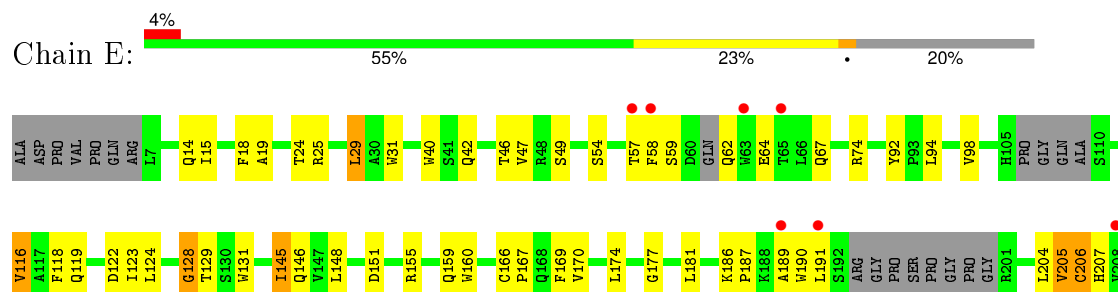
• Molecule 1: Antigen-presenting glycoprotein CD1d

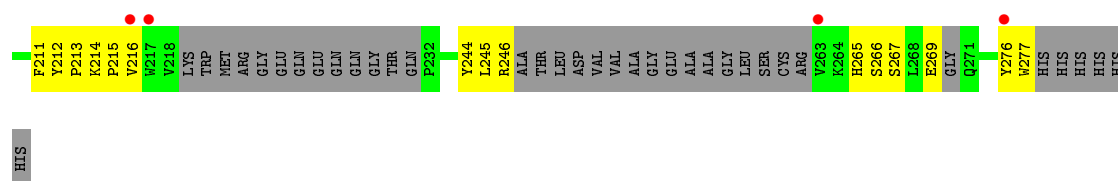


• Molecule 1: Antigen-presenting glycoprotein CD1d

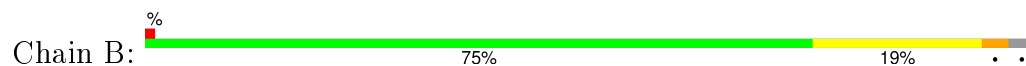


• Molecule 1: Antigen-presenting glycoprotein CD1d

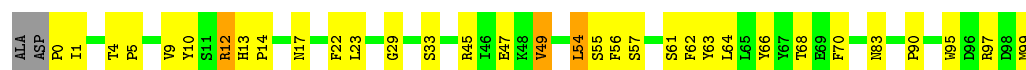




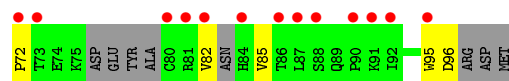
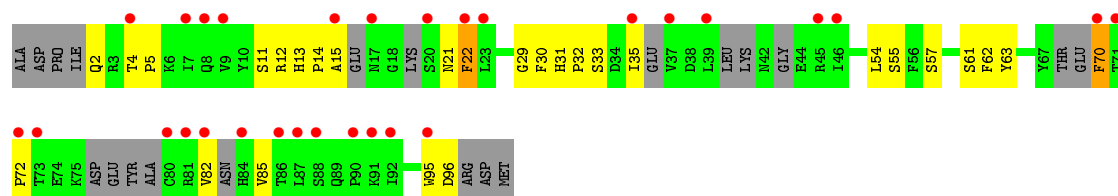
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	108.61Å 127.19Å 332.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.80 46.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (46.03-2.80) 97.3 (46.03-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.213 , 0.259 0.212 , 0.259	Depositor DCC
R_{free} test set	2837 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55792 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8983	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, HEX, NBU, UND, SO4, LSC, FUC

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	0.24	0/2264	0.41	0/3081
1	C	0.23	0/2275	0.42	0/3096
1	E	0.21	0/1894	0.39	0/2571
2	B	0.26	0/851	0.43	0/1152
2	D	0.23	0/859	0.41	0/1163
2	F	0.20	0/649	0.38	0/877
All	All	0.23	0/8792	0.41	0/11940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2198	0	2131	102	0
1	C	2208	0	2139	95	0
1	E	1843	0	1755	64	0
2	B	828	0	794	24	0
2	D	835	0	801	35	0
2	F	636	0	558	30	0
3	A	48	0	43	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	52	20	0
4	C	35	0	52	3	0
5	A	6	0	14	0	0
6	A	15	0	0	2	0
6	C	20	0	0	1	0
6	D	15	0	0	1	0
6	F	5	0	0	1	0
7	A	12	0	16	4	0
7	B	12	0	16	6	0
7	C	6	0	8	1	0
7	D	12	0	16	2	0
8	A	11	0	24	0	0
9	C	34	0	31	8	0
10	E	24	0	22	3	0
11	E	4	0	10	1	0
12	A	58	10	0	6	0
12	B	20	0	0	2	0
12	C	31	0	0	2	0
12	D	10	2	0	1	0
12	E	8	0	0	1	0
12	F	2	0	0	0	0
All	All	8971	12	8482	362	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 22.

The worst 5 of 362 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:A:305:LSC:H12	4:A:305:LSC:H17	1.26	1.16
4:A:305:LSC:H30A	4:A:305:LSC:C22	1.77	1.13
9:C:301:NAG:H4	9:C:303:FUC:H5	1.35	1.07
4:A:305:LSC:H22	4:A:305:LSC:H30A	1.08	1.05
4:A:305:LSC:H22	4:A:305:LSC:C30	1.91	1.00

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	271/284 (95%)	253 (93%)	18 (7%)	0	100	100
1	C	272/284 (96%)	252 (93%)	16 (6%)	4 (2%)	13	40
1	E	214/284 (75%)	201 (94%)	11 (5%)	2 (1%)	21	55
2	B	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
2	D	98/102 (96%)	94 (96%)	4 (4%)	0	100	100
2	F	65/102 (64%)	63 (97%)	2 (3%)	0	100	100
All	All	1017/1158 (88%)	957 (94%)	54 (5%)	6 (1%)	30	65

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	205	VAL
1	C	198	GLY
1	C	21	SER
1	C	179	SER
1	C	128	GLY

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	239/249 (96%)	228 (95%)	11 (5%)	33	67
1	C	240/249 (96%)	234 (98%)	6 (2%)	55	86
1	E	201/249 (81%)	197 (98%)	4 (2%)	63	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	94/96 (98%)	89 (95%)	5 (5%)	28	61
2	D	95/96 (99%)	92 (97%)	3 (3%)	46	80
2	F	67/96 (70%)	64 (96%)	3 (4%)	34	68
All	All	936/1035 (90%)	904 (97%)	32 (3%)	44	78

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	70	PHE
1	C	103	GLU
2	F	4	THR
1	C	35	LEU
1	C	116	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	C	105	HIS
1	C	163	GLN
1	E	265	HIS

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 ⓘ

9 carbohydrates 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	NAG	A	301	1,3	14,14,15	0.67	0	15,19,21	1.89	3 (20%)
3	FUC	A	302	3	10,10,11	0.62	0	14,14,16	1.46	1 (7%)
3	NAG	A	303	3	14,14,15	0.47	0	15,19,21	1.63	2 (13%)
3	FUC	A	304	3	10,10,11	0.67	0	14,14,16	1.21	2 (14%)
9	NAG	C	301	1,9	14,14,15	0.56	0	15,19,21	1.11	2 (13%)
9	FUC	C	302	9	10,10,11	0.55	0	14,14,16	1.95	3 (21%)
9	FUC	C	303	9	10,10,11	0.54	0	14,14,16	1.98	4 (28%)
10	NAG	E	301	1,10	14,14,15	0.51	0	15,19,21	0.71	0
10	FUC	E	302	10	10,10,11	0.66	0	14,14,16	0.92	1 (7%)

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	NAG	A	301	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	302	3	-	0/0/17/20	0/1/1/1
3	NAG	A	303	3	-	0/6/23/26	0/1/1/1
3	FUC	A	304	3	-	0/0/17/20	0/1/1/1
9	NAG	C	301	1,9	-	0/6/23/26	0/1/1/1
9	FUC	C	302	9	-	0/0/17/20	0/1/1/1
9	FUC	C	303	9	-	0/0/17/20	0/1/1/1
10	NAG	E	301	1,10	-	0/6/23/26	0/1/1/1
10	FUC	E	302	10	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	NAG	C1-O5-C5	-5.05	105.84	112.25
3	A	302	FUC	C1-C2-C3	-3.72	105.14	109.54
3	A	304	FUC	C2-C3-C4	-2.37	107.02	111.04
3	A	301	NAG	O3-C3-C4	-2.37	105.01	110.34
10	E	302	FUC	O5-C1-C2	-2.13	107.41	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAG	5	0
3	A	302	FUC	2	0
3	A	303	NAG	4	0
3	A	304	FUC	1	0
9	C	301	NAG	8	0
9	C	303	FUC	7	0
10	E	301	NAG	3	0
10	E	302	FUC	2	0

5.6 Ligand geometry

23 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	$\# Z > 2$
4	LSC	A	305	-	34,34,34	0.85	1 (2%)	37,41,41	0.77	0
5	HEX	A	306	-	5,5,5	0.23	0	4,4,4	0.37	0
6	SO4	A	307	-	4,4,4	0.23	0	6,6,6	0.11	0
6	SO4	A	308	-	4,4,4	0.23	0	6,6,6	0.06	0
6	SO4	A	309	-	4,4,4	0.23	0	6,6,6	0.08	0
7	GOL	A	310	-	5,5,5	0.33	0	5,5,5	0.25	0
7	GOL	A	311	-	5,5,5	0.34	0	5,5,5	0.27	0
8	UND	A	312	-	10,10,10	0.23	0	9,9,9	0.55	0
7	GOL	B	3000	-	5,5,5	0.33	0	5,5,5	0.29	0
7	GOL	B	3001	-	5,5,5	0.38	0	5,5,5	0.26	0
4	LSC	C	304	-	34,34,34	0.86	1 (2%)	37,41,41	0.80	2 (5%)
6	SO4	C	305	-	4,4,4	0.21	0	6,6,6	0.09	0
6	SO4	C	306	-	4,4,4	0.21	0	6,6,6	0.13	0
6	SO4	C	307	-	4,4,4	0.22	0	6,6,6	0.08	0
7	GOL	C	308	-	5,5,5	0.34	0	5,5,5	0.32	0
6	SO4	C	309	-	4,4,4	0.19	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	D	101	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	D	102	-	4,4,4	0.21	0	6,6,6	0.08	0
7	GOL	D	103	-	5,5,5	0.34	0	5,5,5	0.23	0
6	SO4	D	104	-	4,4,4	0.23	0	6,6,6	0.07	0
7	GOL	D	105	-	5,5,5	0.32	0	5,5,5	0.26	0
11	NBU	E	303	-	3,3,3	0.45	0	2,2,2	0.65	0
6	SO4	F	3000	-	4,4,4	0.21	0	6,6,6	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LSC	A	305	-	-	0/36/36/36	0/0/0/0
5	HEX	A	306	-	-	0/3/3/3	0/0/0/0
6	SO4	A	307	-	-	0/0/0/0	0/0/0/0
6	SO4	A	308	-	-	0/0/0/0	0/0/0/0
6	SO4	A	309	-	-	0/0/0/0	0/0/0/0
7	GOL	A	310	-	-	0/4/4/4	0/0/0/0
7	GOL	A	311	-	-	0/4/4/4	0/0/0/0
8	UND	A	312	-	-	0/8/8/8	0/0/0/0
7	GOL	B	3000	-	-	0/4/4/4	0/0/0/0
7	GOL	B	3001	-	-	0/4/4/4	0/0/0/0
4	LSC	C	304	-	-	0/36/36/36	0/0/0/0
6	SO4	C	305	-	-	0/0/0/0	0/0/0/0
6	SO4	C	306	-	-	0/0/0/0	0/0/0/0
6	SO4	C	307	-	-	0/0/0/0	0/0/0/0
7	GOL	C	308	-	-	0/4/4/4	0/0/0/0
6	SO4	C	309	-	-	0/0/0/0	0/0/0/0
6	SO4	D	101	-	-	0/0/0/0	0/0/0/0
6	SO4	D	102	-	-	0/0/0/0	0/0/0/0
7	GOL	D	103	-	-	0/4/4/4	0/0/0/0
6	SO4	D	104	-	-	0/0/0/0	0/0/0/0
7	GOL	D	105	-	-	0/4/4/4	0/0/0/0
11	NBU	E	303	-	-	0/1/1/1	0/0/0/0
6	SO4	F	3000	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	LSC	O19-C18	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	304	LSC	O19-C18	4.08	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	304	LSC	C30-C31-N32	-2.19	108.99	116.03
4	C	304	LSC	O19-C18-C17	2.05	118.15	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	LSC	20	0
6	A	307	SO4	2	0
7	A	310	GOL	2	0
7	A	311	GOL	2	0
7	B	3000	GOL	3	0
7	B	3001	GOL	3	0
4	C	304	LSC	3	0
6	C	306	SO4	1	0
7	C	308	GOL	1	0
7	D	103	GOL	1	0
6	D	104	SO4	1	0
7	D	105	GOL	1	0
11	E	303	NBU	1	0
6	F	3000	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	273/284 (96%)	-0.27	2 (0%) 89 84	31, 52, 100, 140	7 (2%)
1	C	273/284 (96%)	-0.15	1 (0%) 93 90	33, 60, 115, 138	11 (4%)
1	E	226/284 (79%)	0.11	11 (4%) 33 22	47, 100, 140, 174	24 (10%)
2	B	99/102 (97%)	-0.27	1 (1%) 84 77	34, 45, 77, 89	2 (2%)
2	D	100/102 (98%)	-0.28	0 100 100	42, 63, 97, 113	3 (3%)
2	F	82/102 (80%)	1.38	29 (35%) 0 0	67, 122, 152, 168	3 (3%)
All	All	1053/1158 (90%)	-0.03	44 (4%) 40 28	31, 65, 133, 174	50 (4%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	23	LEU	4.8
2	F	82	VAL	4.7
2	F	7	ILE	4.7
2	F	70	PHE	4.3
1	E	217	TRP	4.2

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](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
9	FUC	C	302	10/11	0.89	0.15	-	98,106,109,114	0
10	FUC	E	302	10/11	0.91	0.28	-	127,138,143,143	0
3	NAG	A	303	14/15	0.84	0.27	-	117,124,127,129	0
3	FUC	A	304	10/11	0.86	0.28	-	96,108,124,124	0
10	NAG	E	301	14/15	0.67	0.28	-	123,140,147,149	0
3	NAG	A	301	14/15	0.78	0.17	-	76,100,127,129	0
9	NAG	C	301	14/15	0.88	0.27	-	104,121,135,139	0
9	FUC	C	303	10/11	0.62	0.34	-	148,150,154,156	0
3	FUC	A	302	10/11	0.79	0.33	-	121,141,155,163	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	LSC	C	304	35/35	0.87	0.48	7.28	51,104,183,190	0
7	GOL	A	310	6/6	0.94	0.43	6.09	53,68,80,88	0
8	UND	A	312	11/11	0.92	0.38	5.22	46,53,59,64	0
7	GOL	B	3000	6/6	0.93	0.25	4.85	42,66,82,87	0
5	HEX	A	306	6/6	0.94	0.34	4.59	47,49,58,63	0
11	NBU	E	303	4/4	0.78	0.34	4.50	64,73,76,77	0
4	LSC	A	305	35/35	0.89	0.29	3.92	48,82,149,158	0
6	SO4	C	309	5/5	0.96	0.27	3.20	82,89,91,94	0
6	SO4	C	306	5/5	0.85	0.25	2.66	131,134,137,138	0
7	GOL	A	311	6/6	0.92	0.21	1.37	46,55,58,58	0
6	SO4	D	101	5/5	0.89	0.23	1.19	150,153,155,160	0
6	SO4	A	308	5/5	0.95	0.17	0.37	106,110,113,120	0
6	SO4	C	305	5/5	0.95	0.17	-0.50	98,103,108,121	0
6	SO4	D	102	5/5	0.95	0.14	-0.76	92,95,103,114	0
6	SO4	A	309	5/5	0.81	0.37	-	178,180,181,181	0
7	GOL	D	103	6/6	0.86	0.21	-	82,94,97,101	0
6	SO4	C	307	5/5	0.71	0.33	-	172,174,175,177	0
6	SO4	A	307	5/5	0.94	0.17	-	126,129,134,136	0
7	GOL	C	308	6/6	0.87	0.18	-	72,82,88,89	0
7	GOL	D	105	6/6	0.93	0.18	-	68,76,92,101	0
6	SO4	F	3000	5/5	0.91	0.11	-	124,129,132,134	0
6	SO4	D	104	5/5	0.77	0.24	-	162,164,167,171	0
7	GOL	B	3001	6/6	0.92	0.21	-	61,73,83,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.