

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 07:22 AM BST

PDB ID : 1LK2

Title: 1.35A crystal structure of H-2Kb complexed with the GNYSFYAL peptide

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Deposited on : 2002-04-23

Resolution : 1.35 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 (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 : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.13.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

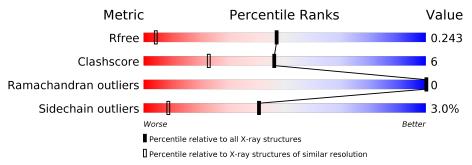
Validation Pipeline (wwPDB-VP) : 2.13.1

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 1.35 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

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 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 <=5%

Mol	Chain	Length	Quality of chain		
1	A	274	88%	11%	-
2	В	99	88%	11%	•
3	Р	8	88%	13%	
4	С	2	100%		

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
8	MRD	В	401	X	_	_	_



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3636 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 H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, K-B ALPHA CHAIN.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	274	Total 2285	C 1448	N 399	O 428	S 10	0	14	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	99	Total 830	C 529	N 138	O 155	S 8	0	3	0

• Molecule 3 is a protein called INSULIN RECEPTOR, BETA-SUBUNIT.

Mol	Chain	Residues	A	A ton	ns		ZeroOcc	AltConf	Trace
3	Р	8	Total 67	C 45	N 9	O 13	0	0	0

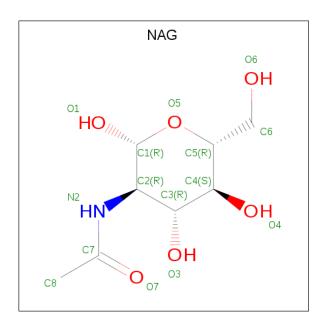
• Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ıs		ZeroOcc	$\mathbf{AltConf}$	Trace
4	С	2	Total 24	C 14	N 1	O 9	0	0	0

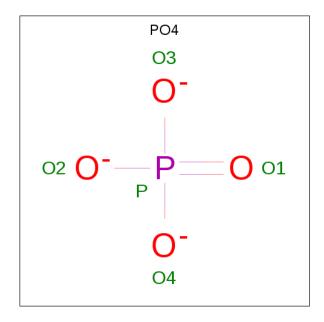
• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
E .	Λ	1	Total	С	N	О	0	0
)	A	1	14	8	1	5	0	0

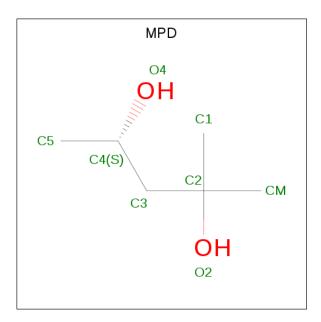
• Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total O : 5 4	P 1	0	0

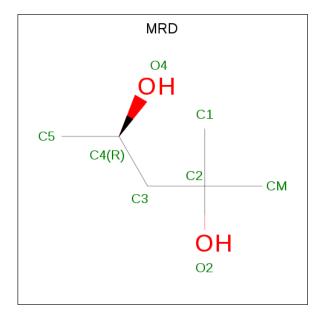
• Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 6 2	0	0
7	В	1	Total C O 8 6 2	0	0

• Molecule 8 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	В	1	Total 8	C 6	O 2	0	0



• Molecule 9 is water.

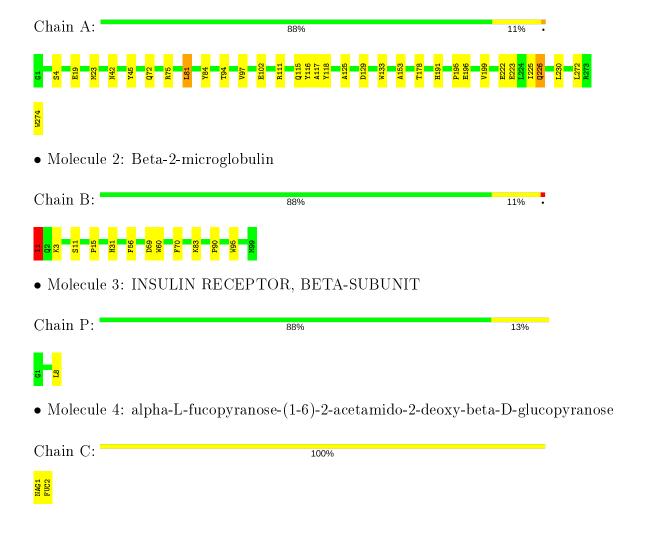
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	284	Total O 284 284	0	0
9	В	96	Total O 96 96	0	0
9	Р	7	Total O 7 7	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, K-B ALPHA CHAIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	135.55Å 87.65Å 45.12Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.35 - 1.35	Depositor
Resolution (A)	18.36 - 1.35	EDS
% Data completeness	93.6 (18.35-1.35)	Depositor
(in resolution range)	92.6 (18.36-1.35)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	1.36 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
D D.	0.149 , 0.164	Depositor
R, R_{free}	0.234 , 0.243	DCC
R_{free} test set	5933 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.53, 68.3	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	0.94	EDS
Total number of atoms	3636	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: PO4, MRD, MPD, NAG, 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	
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	A	0.61	0/2407	0.82	$1/3267 \ (0.0\%)$
2	В	0.58	0/870	0.80	0/1178
3	Р	0.88	0/69	0.84	0/91
All	All	0.61	0/3346	0.81	$1/4536 \ (0.0\%)$

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
2	В	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	129	ASP	CB-CG-OD1	7.06	124.65	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	1	ILE	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	2285	0	2179	29	0
2	В	830	0	800	12	0
3	Р	67	0	59	6	0
4	С	24	0	22	0	0
5	A	14	0	13	0	0
6	A	5	0	0	0	0
7	A	8	0	14	0	0
7	В	8	0	14	4	0
8	В	8	0	14	1	0
9	A	284	0	0	5	0
9	В	96	0	0	2	0
9	Р	7	0	0	0	0
All	All	3636	0	3115	40	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 6.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:11:SER:OG	7:B:403:MPD:H4	1.77	0.85
1:A:81[A]:LEU:HD11	3:P:8:LEU:CD1	2.26	0.66
2:B:15:PRO:HD3	7:B:403:MPD:H52	1.78	0.65
1:A:94[B]:THR:HG23	9:A:3098:HOH:O	1.95	0.65
1:A:81[A]:LEU:CD1	3:P:8:LEU:HD11	2.27	0.65
1:A:226:GLN:HE21	1:A:226:GLN:HA	1.62	0.65
1:A:4[A]:SER:OG	1:A:102:GLU:HG2	1.98	0.63
1:A:81[A]:LEU:CD1	3:P:8:LEU:CD1	2.80	0.60
1:A:191:HIS:CD2	1:A:199[A]:VAL:HG11	2.38	0.59
2:B:3:LYS:NZ	9:B:459:HOH:O	2.35	0.58
1:A:81[A]:LEU:HD13	3:P:8:LEU:HD11	1.86	0.58
1:A:195:PRO:O	1:A:196:GLU:HB2	2.05	0.57
2:B:15:PRO:CD	7:B:403:MPD:H52	2.35	0.57
1:A:81[A]:LEU:HD11	3:P:8:LEU:HD13	1.86	0.56
1:A:81[B]:LEU:HD23	1:A:118:TYR:CD1	2.40	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.42	0.55
1:A:191:HIS:NE2	1:A:199[A]:VAL:HG11	2.23	0.54
9:A:3183:HOH:O	2:B:1:ILE:HG21	2.08	0.54
2:B:95:TRP:CZ2	7:B:403:MPD:H51	2.43	0.53

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
2:B:1:ILE:O	2:B:1:ILE:HG23	2.09	0.53
1:A:72:GLN:HE22	1:A:75:ARG:CZ	2.22	0.53
1:A:178:THR:HG22	9:A:3199:HOH:O	2.10	0.52
1:A:111:ARG:NH1	9:A:3249:HOH:O	2.41	0.51
2:B:1:ILE:O	2:B:1:ILE:CG2	2.58	0.51
1:A:23[A]:MET:SD	8:B:401:MRD:H5C3	2.51	0.50
2:B:3:LYS:NZ	2:B:59:ASP:OD2	2.44	0.50
1:A:81[A]:LEU:HD11	3:P:8:LEU:HD11	1.91	0.49
1:A:223:GLU:HB3	1:A:225:ILE:CD1	2.44	0.48
1:A:226:GLN:HE21	1:A:226:GLN:CA	2.20	0.47
1:A:133:TRP:CZ3	1:A:153:ALA:HB2	2.49	0.47
1:A:81[B]:LEU:HD12	1:A:84:TYR:CD2	2.48	0.47
2:B:83:LYS:HG2	2:B:90:PRO:HG3	1.96	0.47
1:A:19:GLU:OE1	1:A:75:ARG:CZ	2.64	0.46
1:A:115[B]:GLN:HG3	1:A:125:ALA:HB2	1.99	0.45
1:A:116[B]:TYR:HE1	9:A:3245:HOH:O	2.01	0.43
1:A:97:VAL:HG22	1:A:116[B]:TYR:CD2	2.54	0.42
2:B:31:HIS:ND1	9:B:452:HOH:O	2.37	0.42
1:A:195:PRO:O	1:A:196:GLU:CB	2.67	0.41
1:A:133:TRP:HH2	1:A:153:ALA:N	2.19	0.41
1:A:191:HIS:HB2	1:A:274:TRP:CE3	2.57	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	Perce	ntiles
1	A	286/274~(104%)	282 (99%)	4 (1%)	0	100	100
2	В	100/99 (101%)	100 (100%)	0	0	100	100
3	Р	6/8 (75%)	6 (100%)	0	0	100	100
All	All	392/381 (103%)	388 (99%)	4 (1%)	0	100	100



There are no Ramachandran outliers to report.

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	Percei	ntiles
1	A	$246/232 \; (106\%)$	238 (97%)	8 (3%)	38	7
2	В	97/94 (103%)	94 (97%)	3 (3%)	40	8
3	Р	6/6 (100%)	6 (100%)	0	100	100
All	All	349/332 (105%)	338 (97%)	11 (3%)	41	8

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	45	TYR
1	A	81[A]	LEU
1	A	81[B]	LEU
1	A	222	GLU
1	A	226	GLN
1	A	230	LEU
1	A	272	LEU
2	В	1	ILE
2	В	56	PHE
2	В	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	72	GLN
1	A	87	GLN
1	A	174	ASN
1	A	218	GLN
1	A	226	GLN



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)

2 monosaccharides 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).

Mal	Mol Type C		Dog	T in le	Bo	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	NAG	С	1	1,4	14,14,15	0.47	0	17,19,21	1.16	1 (5%)	
4	FUC	С	2	4	10,10,11	0.98	0	14,14,16	2.29	3 (21%)	

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	${f Res}$	Link	Chirals	Torsions	Rings
4	NAG	С	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	С	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
4	С	2	FUC	C1-C2-C3	-6.01	102.28	109.67
4	С	2	FUC	C1-O5-C5	-4.18	103.31	112.78
4	С	2	FUC	O5-C1-C2	3.86	116.73	110.77
4	С	1	NAG	O5-C5-C6	3.61	112.86	107.20



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

5 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	Т	Chain	Dec	Link	Во	ond leng	Bond angles			
MIGI	Type	Chain	m Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2 \mid$
7	MPD	A	402	-	7,7,7	0.46	0	9,10,10	0.79	0
8	MRD	В	401	-	7,7,7	0.44	0	9,10,10	1.29	2 (22%)
6	PO4	A	501	-	4,4,4	0.63	0	6,6,6	0.57	0
5	NAG	A	3001	1	14,14,15	0.46	0	17,19,21	1.43	3 (17%)
7	MPD	В	403	-	7,7,7	0.27	0	9,10,10	1.23	1 (11%)

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
7	MPD	A	402	-	-	3/5/5/5	-
7	MPD	В	403	-	-	0/5/5/5	-
5	NAG	A	3001	1	-	0/6/23/26	0/1/1/1
8	MRD	В	401	-	1/1/2/2	2/5/5/5	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
5	A	3001	NAG	C1-O5-C5	3.24	116.58	112.19

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
5	A	3001	NAG	C4-C3-C2	-2.82	106.88	111.02
5	A	3001	NAG	O5-C1-C2	-2.68	107.05	111.29
8	В	401	MRD	O4-C4-C5	2.53	120.35	109.38
8	В	401	MRD	O4-C4-C3	2.28	120.56	111.36
7	В	403	MPD	O2-C2-CM	2.20	115.13	108.08

All (1) chirality outliers are listed below:

Mol	. (hain	Res	Type	Atom
8		В	401	MRD	C4

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	402	MPD	O2-C2-C3-C4
7	A	402	MPD	CM-C2-C3-C4
8	В	401	MRD	O2-C2-C3-C4
7	A	402	MPD	C2-C3-C4-O4
8	В	401	MRD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	В	401	MRD	1	0
7	В	403	MPD	4	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

