

wwPDB X-ray Structure Validation Summary Report (i)

Feb 3, 2024 – 10:01 AM EST

PDB ID	:	1LBH
Title	:	INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS IN-
		DUCER IPTG
Authors	:	Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.
Deposited on	:	1996-02-17
Resolution	:	3.20 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length		Quality of chain			
1	А	360	38%	32%	11%	•	18%
1	В	360	33%	40%	8%	•	18%
1	С	360	36%	38%	8%	•	18%
1	D	360	35%	35%	10%	•	18%

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
2	IPT	А	400	-	Х	-	-



1LBH

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8932 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 INTACT LACTOSE OPERON REPRESSOR WITH GRA-TUITOUS INDUCER IPTG.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	206	Total	С	Ν	Ο	S	0	0	0
1	Л	290	2218	1383	396	428	11	0	0	0
1	В	206	Total	С	Ν	Ο	S	0	0	0
1	D	290	2218	1383	396	428	11	0	0	0
1	С	206	Total	С	Ν	0	S	0	0	0
	C	290	2218	1383	396	428	11	0	0	0
1	р	206	Total	С	Ν	0	S	0	0	0
1	D	290	2218	1383	396	428	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	109	THR	ALA	conflict	UNP P03023
А	286	LEU	SER	conflict	UNP P03023
В	109	THR	ALA	conflict	UNP P03023
В	286	LEU	SER	conflict	UNP P03023
С	109	THR	ALA	conflict	UNP P03023
С	286	LEU	SER	conflict	UNP P03023
D	109	THR	ALA	conflict	UNP P03023
D	286	LEU	SER	conflict	UNP P03023

• Molecule 2 is 1-methylethyl 1-thio-beta-D-galactopyranoside (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
2	Δ	1	Total	С	0	\mathbf{S}	0	0
2	Π	T	15	9	5	1	0	0
9	В	1	Total	С	Ο	\mathbf{S}	0	0
	D	T	15	9	5	1	0	0
9	С	1	Total	С	Ο	\mathbf{S}	0	0
	U	T	15	9	5	1	0	0
9	Л	1	Total	С	0	S	0	0
	D		15	9	5	1	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.

Note EDS was not executed.

 \bullet Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

Cl	nai	n.	A:	-						38	8%												329	%						119	6	·			189	%	_	_			
MET	PRO	THR	LEU TYR	ASP	VAL	GLU	TYR	ALA GLY	VAL	SER	TYR	THR	VAL	SER	VAL	VAL	ASN	ALA	SER	NAT	SER	ALA	LYS THR	ARG	GLU	VAL	GLU ALA	ALA	MET	GLU	LEU	TYR	ILE	ASN	ARG	VAL	GLN	GLN	LEU ALA	GLY	LYS
SER		1 0 T	T68	L71	A72 173	H74	A75	P76 S77	078	179	V80	A01 A82	I83	K84 cor	R86		L90	492 A92	S93	V94 Vof	V96	297	M98 Vqq	E100	R101	6103	V104 E105	A106	C107	A110	V111	N113	L114 1115	0111	R118	V119 8120	G121	L122	Y126	P127	L128
D130	D132	V136	C140	T141	N142 V143	P144	A145	L146	V150	<mark>S151</mark>	D152	4153 T154	P155	I156 N167	ICTN .	F161	S162 1122	C0 1U	R168	L169 C170	V171	E172	H173 1174		L177	H179	4183	L184	D1 00		S191	L196	R197		K2 <mark>03</mark>	TOCE	R207		E215 R216		D219
2002	G225 8225	0227 0227	0228 T229	M230	<mark>Q231</mark>	M242		A245 N246	D247	Q248	M249	A 250 L 251	-	M254 DDEE	A256		V264	4203 A266		S269	Y273	D274	D275 T976		C281	1 202 I 283	P284 P285	L286	T287	1200 1289	K290	TGZħ	L296	0298 0298		V301	R303	L304	L305 0306	L307	
Q311 A312	V313	G315	N316 D317		5322 1323	V324	K325	R326 K327	T328	T329	L330	P332	N333	T334	T336	A337	S338 D220	R340	A341	L342	D344	S345	L346 M347	Q348	L349	R351	Q352 V353	S354	R355	E357	SER GT V	GLN									
•	М	hle	CII	le	1		IN	гı	٦Δ	\mathbf{C}	!T	T	. Δ	۱C	'T	'n	SI	F)	\cap	P	El	R(יכ	J.	RI	EF	PR	E	SS	0	R	v	VI	тı	H	G	R	\mathbf{A}'	ті	T	т

• Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

С	ha	ai	n	В	:							33	%														4	109	%								8	3%		•			18	8%	þ						
MET	LYS	VAL	THR	LEU	TYR	ASP	AI.A	GLU	TYR	ALA	GLY	VAL	SER	TYR	THP	VAL.	SER	ARG	VAL	VAL	ASN	GLN	ALA	NEK		SER	ALA	LYS	THR	ARG	GLU	VAL	CLU	ALA	ALA	MET	GI.II	TEU	ASN	TYR	ILE	ASN	ARG	VAL	ALA	GLN	UEU I'EU	ALA	GLY	LYS	GLN
SER	L62	164 164		T68	S69	S70		H74	A75	P76	S77	Q78	6/1	V80		183 183	K84	<u>585</u>	R86	A87	D88	089	L90	cuo cuo	CEC DOV	V 95	06N	297	M98	060 N	E100	R101	G103	V104	E105	A106	K108	T109	A110	V111	111	L115	A116	Q117	R118	V119	6121		N125	Y126	P127
L128	D129	0131	D132		V136	E137	A139	C140	-	V143		L146	F147	L148	0153		P155	I156	N157	S158	I159	1160	F161	7919	T167	R168	-	V171		L174	V175	A1 / O		Q180		L185	P188	L189	S190	S191	V192	A194	R195	L196	R197	L198	W201		Y204		N208
Q 209	1210	P212	1213	A214	E215	R216	D219		A222	M223	S224	G225		<mark>1228</mark>	1229 M930	0231	M232	-	1237	V238	P239	T240	A241	M242	L240	N246	D247	<mark>Q248</mark>	M249	A250	L251	4202 4753	M264	R255	A256	1257 TOE9	F.259	S260	G261	L262	R263		<mark>\$269</mark>	V270	V271	G272	12/3 D274	D275	T276		S280



V353 S354 R355 L356 L356 E357 SER GLY GLN

 \bullet Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

Chain	C:	36%	38%	8% •	18%
MET LYS PRO VAL THR	LEU TYR ASP VAL ALA GLU TYR ALA GLV GLY	VAL VAL TYR TTR THR VAL VAL VAL ASN VAL ASN VAL ASN VAL ASN VAL ASN VAL	ALA THR ARG ARG GLU CYS CVAL CYS GLU ALA ALA	GLU LEU ASN TYR TLE PRO ASN	ARG ALA ALA GLN GLN LEU LVS GLN GLN
SER L62 L63	869 870 870 870 872 876 877 877	078 179 179 1886 1886 1988 1986 1989 1984 1984 1984 1986 1986 1986 1986 1986	V99 E100 R101 S102 G103 V104 E105 A106 C107 K108 H112	L114 L114 Q117 R118 V119	L122 1133 1123 1128 1128 1128 0130 0130 0130
A133 1134 C140 T141	N142 N144 P144 P144 L146 F146 F146 L148 D1498 V150	8151 8152 9152 1154 1154 1156 1156 1156 1156 1156 1161 1174 1173 1174 1173 1174 1174 1174 117	H179 4180 1184 1184 1188 1188 1188 1189 1191 1189	L196 R197 L198 W201 H202	1206 1210 1210 1211 1213 1213 1213
D219 W220 S224 C225	F226 Q227 Q228 M230 Q231 Q231 L233 L233	P239 1240 A241 M242 V244 V244 A245 A245 A245 A265 A265 A265 A265 A265 A265 A265 A26	1258 8259 1264 1267 1267 1271 1272 1273 1274	D275 T276 E277 D278 S279 S279 C281	Y282 P286 P286 P286 F286 T286 T286 Y289 Y290 Q291
L296 G297 Q298	R303 L304 L305 Q306 L307 S308 G310 G310 Q310	A312 V313 K313 K314 K316 C316 C315 K325 K326 K327 T329 K327 T329 K331 F3332 F332 F332 F3322 F3322 F3322 F3322 F3322 F3322 F3322 F3322 F3322 F3322 F332 F32 F	1334 1335 1337 1337 1337 1333 1333 1333 1334 1343 1343	L346 M347 Q348 L349 A350 R351 Q352	V353 S354 L355 E357 GLY GLN
• Mole IPTG	ecule 1: INT	ACT LACTOSE OPEF	RON REPRESS	OR WITI	H GRATUITOUS INDUCER
Chain	D:	35%	35% 10	•	18%
MET LYS PRO VAL THR	LEU TYR ASP VAL ALA GLU GLU GLV GLY	VAL TYPR THR THR CLN CLN CLN VAL ANC ANC ANC ANC ANC ANC ANC ANC ANC ANC	ALA LYS THR ARG GLU CYS VAL CYS GLU ALA ALA ALA	GLU LEU ASN TYR ILE PRO ASN	ARG ALA ALA ALA CLN CLN CLN CLN CLN CLN CLY CLY CLY CLY CLY
SER L62 L63 L64	869 870 876 179 180 183	K84 886 R86 R86 R86 R86 R86 083 198 089 893 V95 V95 V95 V95 V95 V95 S93 S100	E105 A106 L114 L115 A115 A115 A115 A117 V119 V119 V119 V121	L122 1123 1123 1126 1127 D129 D129	D130 0131 0132 132 136 136 136 136 136 140 1140 1141
V143 P144 A145 L146 F147	L148 D149 V150 S151 D152 D153 D153 T156 N157	8158 1169 1166 1165 1167 1167 1167 1167 1167 1171 1172 1172	(181 1184 1185 1185 1185 1188 8191 8191 8192 8192 8192 8194	R195 L196 R197 G200 W201	Y204 1205 7205 7207 7207 7210 7211 7210 7211
A214 V143 E215 P144 R216 A145 L146 D219 F147	W220 1148 W220 1149 Q228 1150 T229 8151 Q231 Q152 Q231 Q153 M232 1155 M234 N157	E255 5158 1236 1160 1237 1160 1238 1160 P239 0165 P240 0166 A241 1167 A241 1167 A245 1169 A245 1166 A245 1167 A245 1167 A245 1171 A245 1171 A245 1172 A245 1171 A245 1173 A245 <td>A255 1181 A255 1184 1257 1184 1259 1185 259 1185 259 1186 259 1186 259 1186 259 1186 259 1186 256 3191 256 3191 256 3191 256 3191 256 3191 256 3191 2565 3191 2565 3191 2565 3191</td> <td>S269 8195 11196 1272 8197 1273 1197 1274 1197 1263 1120</td> <td>P284 Y204 P285 L205 L286 L205 L287 N201 T288 Q209 Q297 Q211 Q298 P213 Q291 1210 Q293 P213 Q294 P213</td>	A255 1181 A255 1184 1257 1184 1259 1185 259 1185 259 1186 259 1186 259 1186 259 1186 259 1186 256 3191 256 3191 256 3191 256 3191 256 3191 256 3191 2565 3191 2565 3191 2565 3191	S269 8195 11196 1272 8197 1273 1197 1274 1197 1263 1120	P284 Y204 P285 L205 L286 L205 L287 N201 T288 Q209 Q297 Q211 Q298 P213 Q291 1210 Q293 P213 Q294 P213



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants	141.20Å 75.10Å 149.20Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 - 3.20	Depositor
% Data completeness	(Not available) $(15.00-3.20)$	Depositor
(in resolution range)	(100 available) (10.00 0.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8932	wwPDB-VP
Average B, all atoms $(Å^2)$	9.0	wwPDB-VP



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: IPT

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		Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.72	1/2247~(0.0%)	0.92	4/3055~(0.1%)	
1	В	0.72	1/2247~(0.0%)	0.94	1/3055~(0.0%)	
1	С	0.73	0/2247	0.93	2/3055~(0.1%)	
1	D	0.78	1/2247~(0.0%)	0.96	7/3055~(0.2%)	
All	All	0.74	3/8988~(0.0%)	0.94	14/12220~(0.1%)	

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	С	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	D	230	MET	SD-CE	-9.74	1.23	1.77
1	А	281	CYS	CB-SG	-6.41	1.71	1.82
1	В	107	CYS	CB-SG	-5.40	1.73	1.81

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	283	ILE	C-N-CD	7.56	144.28	128.40
1	D	283	ILE	C-N-CD	6.49	142.04	128.40
1	D	236	GLY	N-CA-C	6.37	129.03	113.10
1	D	356	LEU	CA-CB-CG	6.25	129.67	115.30
1	D	287	THR	N-CA-C	-6.17	94.35	111.00



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	126	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2218	0	2269	157	1
1	В	2218	0	2269	177	0
1	С	2218	0	2269	178	0
1	D	2218	0	2269	147	0
2	А	15	0	17	0	0
2	В	15	0	14	3	0
2	С	15	0	16	1	0
2	D	15	0	17	0	0
All	All	8932	0	9140	602	1

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 33.

The worst 5 of 602 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)
1:B:213:ILE:HD11	1:B:239:PRO:HB3	1.23	1.17
1:D:283:ILE:HG22	1:D:284:PRO:HD3	1.23	1.17
1:A:283:ILE:HG12	1:B:283:ILE:HD12	1.29	1.09
1:C:144:PRO:HG2	1:C:308:SER:HA	1.50	0.93
1:D:283:ILE:HG22	1:D:284:PRO:CD	1.98	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)	
1:A:334:THR:O	1:A:334:THR:O[2_555]	2.19	0.01	



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	entiles
1	А	294/360~(82%)	237 (81%)	41 (14%)	16 (5%)	2	14
1	В	294/360~(82%)	231 (79%)	41 (14%)	22 (8%)	1	7
1	С	294/360~(82%)	244 (83%)	33 (11%)	17 (6%)	1	13
1	D	294/360~(82%)	242 (82%)	31 (10%)	21 (7%)	1	8
All	All	1176/1440 (82%)	954 (81%)	146 (12%)	76 (6%)	1	10

5 of 76 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	101	ARG
1	А	142	ASN
1	А	274	ASP
1	А	283	ILE
1	А	312	ALA

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	Pe	erce	entil	$\overline{\mathbf{es}}$
1	А	243/295~(82%)	199 (82%)	44 (18%)		1	8	
1	В	243/295~(82%)	206 (85%)	37 (15%)		3	13	
1	С	243/295~(82%)	210 (86%)	33 (14%)		3	17	
1	D	243/295~(82%)	200 (82%)	43 (18%)		2	9	
All	All	972/1180~(82%)	815 (84%)	157 (16%)		2	11	



5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	D	63	LEU
1	D	264	VAL
1	D	102	SER
1	D	156	ILE
1	D	324	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	163	HIS
1	С	348	GLN
1	D	306	GLN
1	С	335	GLN
1	D	153	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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).



Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	IPT	А	400	-	14,15,15	3.64	8 (57%)	18,21,21	4.12	16 (88%)
2	IPT	С	400	-	14,15,15	3.41	7 (50%)	18,21,21	4.34	12 (66%)
2	IPT	В	400	-	14,15,15	<mark>3.30</mark>	6 (42%)	18,21,21	<mark>3.41</mark>	11 (61%)
2	IPT	D	400	-	14,15,15	3.67	5 (35%)	18,21,21	3.75	10 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IPT	А	400	-	-	5/6/26/26	0/1/1/1
2	IPT	С	400	-	-	0/6/26/26	0/1/1/1
2	IPT	В	400	-	-	4/6/26/26	0/1/1/1
2	IPT	D	400	-	-	5/6/26/26	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	400	IPT	C1'-S1	-8.34	1.46	1.83
2	D	400	IPT	C1'-S1	-7.97	1.48	1.83
2	В	400	IPT	C1'-S1	-7.84	1.49	1.83
2	С	400	IPT	C1'-S1	-7.53	1.50	1.83
2	А	400	IPT	O5-C1	7.13	1.53	1.42

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	400	IPT	O5-C1-C2	8.21	120.64	110.31
2	А	400	IPT	O3-C3-C2	-7.80	92.32	110.35
2	С	400	IPT	O5-C5-C4	-7.44	96.18	109.69
2	С	400	IPT	C1-O5-C5	7.13	125.73	112.58
2	А	400	IPT	O5-C1-C2	6.80	118.86	110.31

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	400	IPT	O5-C1-S1-C1'
2	А	400	IPT	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
2	А	400	IPT	C3'-C1'-S1-C1
2	В	400	IPT	O5-C1-S1-C1'
2	D	400	IPT	O5-C1-S1-C1'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	400	IPT	1	0
2	В	400	IPT	3	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

