W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 09:57 AM BST

PDB ID	:	1LOA
Title	:	THREE-DIMENSIONAL STRUCTURES OF COMPLEXES OF LATH-YRUS OCHRUS ISOLECTIN I WITH GLUCOSE AND MANNOSE: FINE SPECIFICITY OF THE MONOSACCHARIDE-BINDING SITE
Authors	:	Bourne, Y.; Cambillau, C.
Deposited on	:	1993-01-27
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references ⓘ) 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 2.20 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.
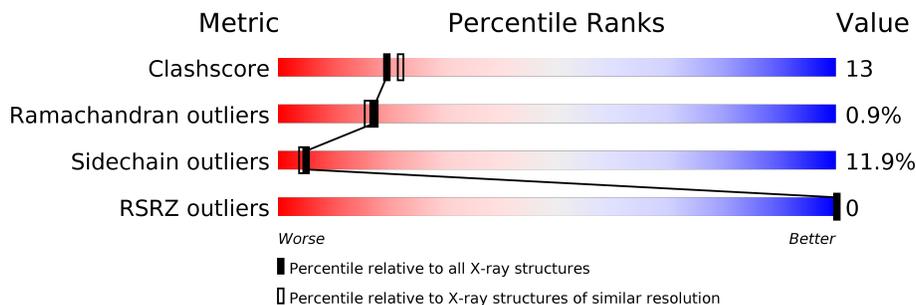
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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% 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	181	62% 31% 6% ·
1	C	181	64% 28% 8% ··
1	E	181	60% 30% 5% · ·
1	G	181	59% 33% 7% ··
2	B	52	67% 23% 10%
2	D	52	65% 19% 6% 10%
2	F	52	50% 37% · 10%

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Mol	Chain	Length	Quality of chain
2	H	52	54%　　　　　　　　33%　　・　10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7460 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 LEGUME ISOLECTIN I (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	180	Total 1397	C 890	N 230	O 277	0	0	0
1	C	180	Total 1397	C 890	N 230	O 277	0	0	0
1	E	180	Total 1397	C 890	N 230	O 277	0	0	0
1	G	180	Total 1397	C 890	N 230	O 277	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	LYS	conflict	UNP P04122
C	153	ALA	LYS	conflict	UNP P04122
E	153	ALA	LYS	conflict	UNP P04122
G	153	ALA	LYS	conflict	UNP P04122

- Molecule 2 is a protein called LEGUME ISOLECTIN I (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total 381	C 251	N 58	O 72	0	0	0
2	D	47	Total 376	C 248	N 58	O 70	0	0	0
2	F	47	Total 381	C 251	N 58	O 72	0	0	0
2	H	47	Total 376	C 248	N 58	O 70	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	TYR	PHE	conflict	UNP P12306
D	41	TYR	PHE	conflict	UNP P12306
F	41	TYR	PHE	conflict	UNP P12306
H	41	TYR	PHE	conflict	UNP P12306

- Molecule 3 is methyl alpha-D-glucopyranoside (three-letter code: GYP) (formula: $C_7H_{14}O_6$).
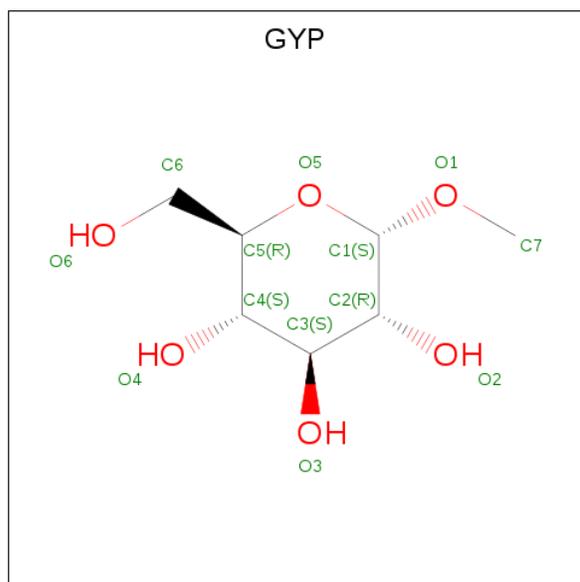
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	7	6		
3	C	1	Total	C	O	0	0
			13	7	6		
3	E	1	Total	C	O	0	0
			13	7	6		
3	G	1	Total	C	O	0	0
			13	7	6		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Ca 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Mn 1	0	0
5	A	1	Total 1	Mn 1	0	0
5	C	1	Total 1	Mn 1	0	0
5	F	1	Total 1	Mn 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total 73	O 73	0	0
6	B	17	Total 17	O 17	0	0
6	C	59	Total 59	O 59	0	0
6	D	8	Total 8	O 8	0	0
6	E	53	Total 53	O 53	0	0
6	F	9	Total 9	O 9	0	0
6	G	70	Total 70	O 70	0	0
6	H	9	Total 9	O 9	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)
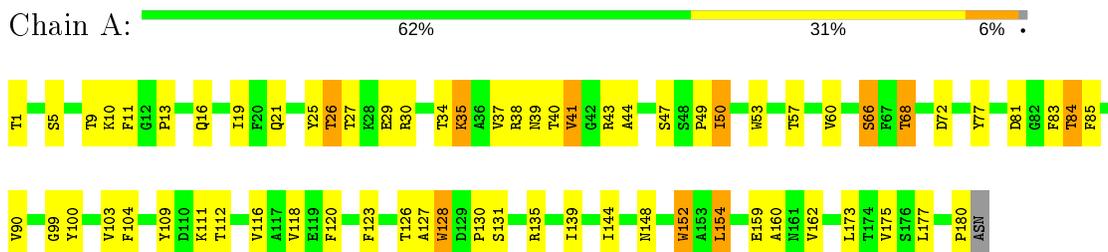
Chain A:

- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain C:

- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain E:

- Molecule 1: LEGUME ISOLECTIN I (ALPHA CHAIN)

Chain G:

T96 G97 L101 G102 V103 F104 N105 S106 Y109 D110 S113 Q114 T115 V116 A117 W128 D129 P130 S131 N132 G133 D134 R135 H136 D140 V141 N142 S143 T149 K150 S151 W152 E159 A160 N161 V162 N167 A168 A169 T170 N171 V172 L177 T178 Y179 P180 ASN

• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain B:

| 67% | 23% | 10% |

E1 T5 V10 P11 L12 V16 W19 T27 T28 A33 A34 H35 W40 Y41 L46 A47 GLY THR SER SER

• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain D:

| 65% | 19% | 6% | 10% |

GLU T2 S3 E8 V9 V10 P17 E18 W19 V20 R21 T27 E36 V37 W40 Y41 E45 G48 THR SER SER

• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain F:

| 50% | 37% | • | 10% |

E1 Y4 T5 L6 P11 L12 K13 E14 F15 V16 P17 E18 W19 V20 R21 S25 E31 F32 A33 A34 H35 W40 Y41 F42 H43 S44 A47 GLY THR SER SER

• Molecule 2: LEGUME ISOLECTIN I (BETA CHAIN)

Chain H:

| 54% | 33% | • | 10% |

GLU T2 T5 L6 N7 E8 V9 V10 P11 E14 W19 V20 R21 T27 E31 H35 L38 S39 W40 Y41 F42 L46 A47 G48 THR SER SER
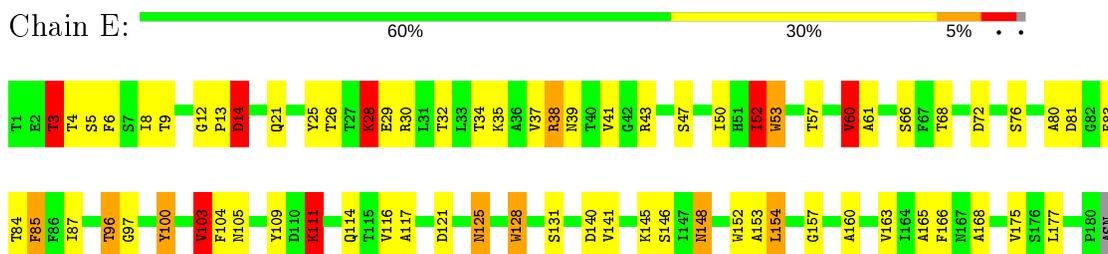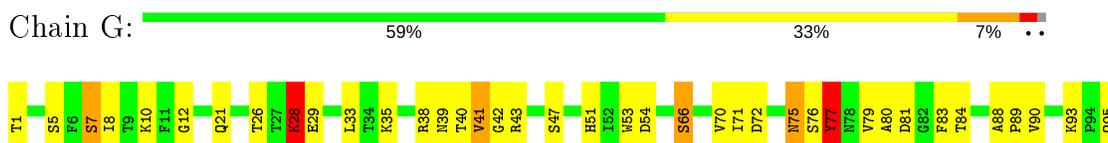
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.30Å 139.80Å 62.70Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 7.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.20) 67.2 (7.99-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 71.8	EDS
L-test for twinning[1]	$<\lvert L\rvert> = 0.46, <L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7460	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $<\lvert L\rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MN, GYP

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	1.04	0/1431	1.82	34/1954 (1.7%)
1	C	0.96	0/1431	1.83	30/1954 (1.5%)
1	E	1.01	1/1431 (0.1%)	1.85	32/1954 (1.6%)
1	G	0.99	1/1431 (0.1%)	1.76	18/1954 (0.9%)
2	B	1.17	0/394	1.75	7/539 (1.3%)
2	D	1.03	0/389	1.84	9/532 (1.7%)
2	F	1.13	0/394	1.91	9/539 (1.7%)
2	H	1.17	0/389	1.81	9/532 (1.7%)
All	All	1.03	2/7290 (0.0%)	1.82	148/9958 (1.5%)

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	E	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	116	VAL	CA-CB	6.01	1.67	1.54
1	E	60	VAL	CA-CB	5.81	1.67	1.54

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4	TYR	CB-CG-CD1	-13.97	112.62	121.00
2	H	41	TYR	CB-CG-CD1	-10.87	114.48	121.00
1	E	152	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	C	172	VAL	CG1-CB-CG2	-9.20	96.18	110.90
1	E	100	TYR	CB-CG-CD1	-9.06	115.56	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	41	TYR	Sidechain
1	E	25	TYR	Sidechain
2	F	4	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1397	0	1346	29	0
1	C	1397	0	1346	29	0
1	E	1397	0	1346	44	0
1	G	1397	0	1346	40	0
2	B	381	0	357	6	0
2	D	376	0	351	8	0
2	F	381	0	357	21	0
2	H	376	0	351	20	0
3	A	13	0	14	0	0
3	C	13	0	14	3	0
3	E	13	0	14	1	0
3	G	13	0	14	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	1	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	73	0	0	2	0
6	B	17	0	0	2	0
6	C	59	0	0	3	0
6	D	8	0	0	0	0
6	E	53	0	0	2	0
6	F	9	0	0	0	0
6	G	70	0	0	2	0
6	H	9	0	0	0	0
All	All	7460	0	6856	160	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 13.

The worst 5 of 160 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:C:130:PRO:HG3	1:C:149:THR:HG21	1.51	0.92
1:E:84:THR:HG21	1:E:117:ALA:HB1	1.57	0.83
1:A:21:GLN:HE22	1:A:43:ARG:HH21	1.31	0.75
1:A:10:LYS:HD2	1:A:29:GLU:HB3	1.73	0.70
1:C:122:THR:HA	1:C:135:ARG:HG2	1.75	0.69

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	178/181 (98%)	172 (97%)	5 (3%)	1 (1%)	25	26
1	C	178/181 (98%)	164 (92%)	13 (7%)	1 (1%)	25	26
1	E	178/181 (98%)	165 (93%)	11 (6%)	2 (1%)	14	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	178/181 (98%)	164 (92%)	10 (6%)	4 (2%)	6	4
2	B	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
2	D	45/52 (86%)	44 (98%)	1 (2%)	0	100	100
2	F	45/52 (86%)	41 (91%)	4 (9%)	0	100	100
2	H	45/52 (86%)	43 (96%)	2 (4%)	0	100	100
All	All	892/932 (96%)	836 (94%)	48 (5%)	8 (1%)	17	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	28	LYS
1	C	28	LYS
1	G	39	ASN
1	E	28	LYS
1	E	111	LYS

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	Percentiles	
1	A	154/155 (99%)	135 (88%)	19 (12%)	4	4
1	C	154/155 (99%)	137 (89%)	17 (11%)	6	5
1	E	154/155 (99%)	130 (84%)	24 (16%)	2	2
1	G	154/155 (99%)	128 (83%)	26 (17%)	2	1
2	B	40/44 (91%)	40 (100%)	0	100	100
2	D	39/44 (89%)	37 (95%)	2 (5%)	24	29
2	F	40/44 (91%)	37 (92%)	3 (8%)	13	14
2	H	39/44 (89%)	38 (97%)	1 (3%)	46	58
All	All	774/796 (97%)	682 (88%)	92 (12%)	5	4

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	28	LYS
1	E	68	THR
1	G	116	VAL
1	E	29	GLU
1	E	38	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	21	GLN
1	E	125	ASN
1	G	75	ASN
1	C	142	ASN
1	E	16	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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	GYP	C	182	-	13,13,13	0.80	0	18,18,18	1.65	3 (16%)
3	GYP	E	182	-	13,13,13	0.97	1 (7%)	18,18,18	1.67	4 (22%)
3	GYP	G	182	-	13,13,13	0.71	0	18,18,18	1.14	1 (5%)
3	GYP	A	182	-	13,13,13	0.92	0	18,18,18	1.67	4 (22%)

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	GYP	C	182	-	-	1/4/24/24	0/1/1/1
3	GYP	E	182	-	-	2/4/24/24	0/1/1/1
3	GYP	G	182	-	-	1/4/24/24	0/1/1/1
3	GYP	A	182	-	-	0/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	182	GYP	O1-C1	2.04	1.43	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	182	GYP	C6-C5-C4	-4.41	102.67	113.00
3	C	182	GYP	C4-C3-C2	-4.32	103.28	110.82
3	A	182	GYP	C7-O1-C1	-4.22	106.77	113.27
3	C	182	GYP	O1-C1-C2	-3.47	104.08	108.15
3	E	182	GYP	C4-C3-C2	-3.37	104.94	110.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	182	GYP	O5-C1-O1-C7
3	G	182	GYP	O5-C1-O1-C7
3	E	182	GYP	O5-C5-C6-O6
3	E	182	GYP	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	182	GYP	3	0
3	E	182	GYP	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(Å²)	Q<0.9
1	A	180/181 (99%)	-1.07	0	100	100	11, 22, 35, 48	0
1	C	180/181 (99%)	-0.87	0	100	100	12, 30, 46, 57	0
1	E	180/181 (99%)	-0.89	0	100	100	13, 27, 44, 57	0
1	G	180/181 (99%)	-0.99	0	100	100	16, 26, 41, 51	0
2	B	47/52 (90%)	-1.13	0	100	100	6, 21, 31, 46	0
2	D	47/52 (90%)	-1.04	0	100	100	12, 28, 38, 41	0
2	F	47/52 (90%)	-1.01	0	100	100	9, 29, 41, 49	0
2	H	47/52 (90%)	-1.07	0	100	100	15, 23, 33, 39	0
All	All	908/932 (97%)	-0.98	0	100	100	6, 26, 42, 57	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	A	228	1/1	0.82	0.10	27,27,27,27	0
5	MN	F	689	1/1	0.85	0.32	29,29,29,29	0
3	GYP	C	182	13/13	0.92	0.10	40,43,46,49	0
3	GYP	E	182	13/13	0.93	0.10	32,38,45,46	0
4	CA	E	688	1/1	0.96	0.08	56,56,56,56	0
3	GYP	G	182	13/13	0.96	0.08	27,30,32,34	0
4	CA	C	458	1/1	0.96	0.15	36,36,36,36	0
5	MN	C	459	1/1	0.97	0.04	41,41,41,41	0
4	CA	G	918	1/1	0.97	0.06	33,33,33,33	0
3	GYP	A	182	13/13	0.97	0.08	18,22,25,28	0
5	MN	G	919	1/1	0.98	0.04	28,28,28,28	0
5	MN	A	229	1/1	0.99	0.03	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.