



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:58 AM UTC

PDB ID : 3FS1 / pdb_00003fs1
Title : Crystal structure of HNF4a LBD in complex with the ligand and the coactivator PGC-1a fragment
Authors : Rha, G.; Wu, G.; Chi, Y.
Deposited on : 2009-01-08
Resolution : 2.20 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

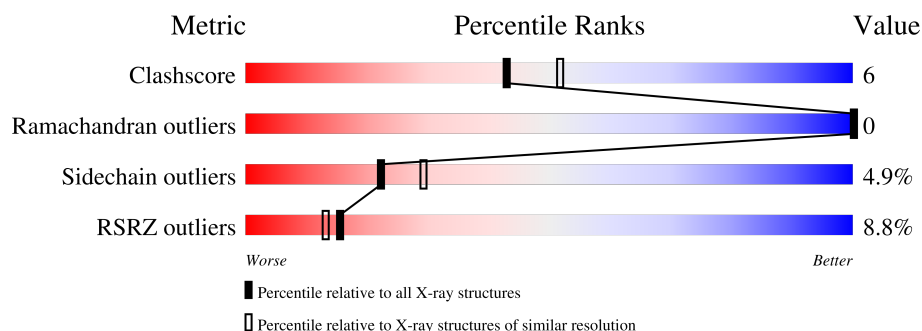
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	230	7% 67% 27% 5%
2	B	9	67% 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1973 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.

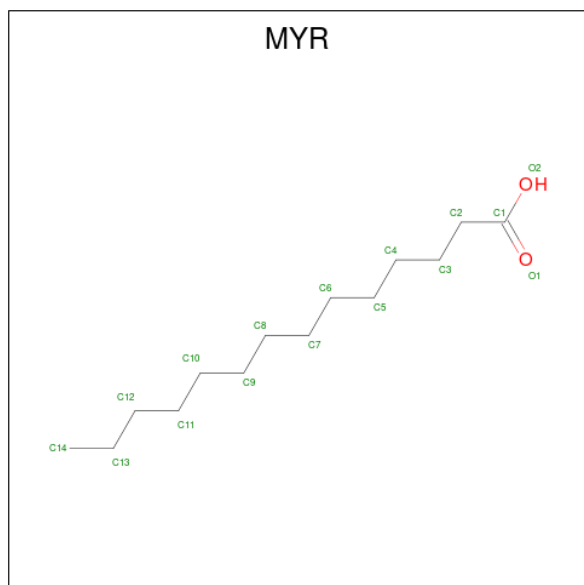
- Molecule 1 is a protein called Hepatocyte nuclear factor 4-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1825	1172	306	338	9			

- Molecule 2 is a protein called PPARGgamma Coactivator-1a (PGC-1a).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			55	36	9	10			

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	14	2		

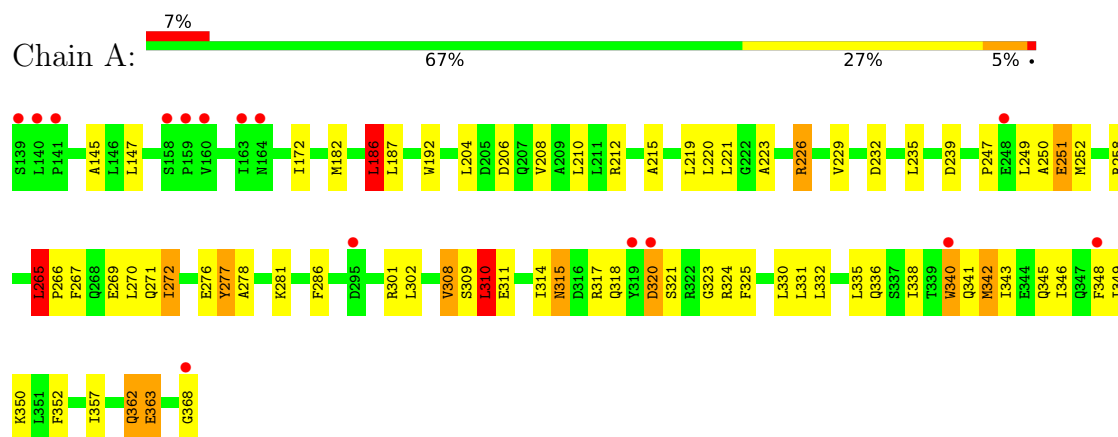
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		

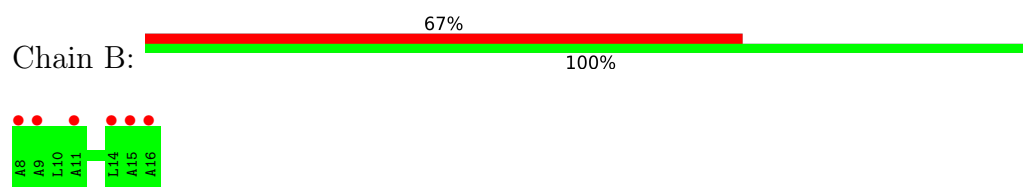
3 Residue-property plots

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: Hepatocyte nuclear factor 4-alpha



- Molecule 2: PPARgamma Coactivator-1a (PGC-1a)



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.05Å 113.05Å 57.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (40.00-2.20) 98.2 (40.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.236 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1973	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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, 0.333 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: MYR

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	2.10	50/1855 (2.7%)	1.53	18/2507 (0.7%)
2	B	1.29	0/54	0.84	0/72
All	All	2.08	50/1909 (2.6%)	1.52	18/2579 (0.7%)

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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	LEU	N-CA	-12.81	1.35	1.46
1	A	258	ARG	CD-NE	-11.64	1.29	1.46
1	A	251	GLU	CB-CG	-11.42	1.18	1.52
1	A	226	ARG	CD-NE	-8.73	1.34	1.46
1	A	182	MET	SD-CE	-8.45	1.58	1.79
1	A	346	ILE	CA-CB	-8.44	1.44	1.54
1	A	145	ALA	CA-C	8.25	1.63	1.52
1	A	342	MET	SD-CE	7.89	1.99	1.79
1	A	310	LEU	CA-C	-7.22	1.43	1.52
1	A	338	ILE	CA-CB	-6.83	1.46	1.54
1	A	172	ILE	N-CA	-6.69	1.37	1.46
1	A	343	ILE	CA-C	6.68	1.61	1.52
1	A	309	SER	C-O	-6.60	1.15	1.24
1	A	215	ALA	CA-C	6.58	1.61	1.52
1	A	348	PHE	CA-C	6.54	1.61	1.52
1	A	272	ILE	CA-CB	6.45	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	GLN	N-CA	-6.44	1.38	1.46
1	A	250	ALA	C-N	-6.30	1.25	1.33
1	A	278	ALA	CA-CB	-6.30	1.43	1.53
1	A	343	ILE	CA-CB	-6.27	1.46	1.54
1	A	276	GLU	C-O	-6.12	1.17	1.24
1	A	330	LEU	C-O	-6.07	1.16	1.24
1	A	271	GLN	CA-CB	6.01	1.62	1.53
1	A	172	ILE	C-O	-5.99	1.18	1.24
1	A	286	PHE	C-O	-5.88	1.17	1.23
1	A	323	GLY	C-O	-5.88	1.16	1.24
1	A	357	ILE	CA-CB	5.87	1.60	1.53
1	A	311	GLU	C-O	-5.83	1.16	1.24
1	A	277	TYR	N-CA	-5.79	1.39	1.46
1	A	336	GLN	CG-CD	5.64	1.66	1.52
1	A	223	ALA	CA-CB	-5.60	1.44	1.53
1	A	258	ARG	C-O	-5.55	1.17	1.24
1	A	362	GLN	C-O	-5.54	1.17	1.24
1	A	325	PHE	N-CA	-5.51	1.39	1.46
1	A	235	LEU	C-O	5.45	1.30	1.24
1	A	338	ILE	N-CA	-5.44	1.40	1.46
1	A	187	LEU	C-O	-5.35	1.17	1.24
1	A	229	VAL	CA-CB	5.32	1.60	1.54
1	A	206	ASP	N-CA	-5.26	1.39	1.46
1	A	269	GLU	N-CA	-5.22	1.40	1.46
1	A	186	LEU	CA-CB	-5.19	1.45	1.53
1	A	308	VAL	N-CA	-5.19	1.40	1.46
1	A	315	ASN	C-O	-5.17	1.17	1.24
1	A	331	LEU	C-O	-5.15	1.17	1.24
1	A	269	GLU	C-O	-5.12	1.18	1.24
1	A	258	ARG	N-CA	-5.12	1.40	1.46
1	A	247	PRO	C-O	-5.11	1.17	1.24
1	A	265	LEU	C-O	-5.10	1.19	1.24
1	A	265	LEU	N-CA	-5.07	1.41	1.46
1	A	335	LEU	N-CA	-5.07	1.40	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLU	CB-CG-CD	-13.13	90.27	112.60
1	A	251	GLU	CA-CB-CG	11.36	136.81	114.10
1	A	251	GLU	N-CA-C	10.91	126.10	113.01
1	A	226	ARG	NE-CZ-NH2	-9.56	110.60	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	NE-CZ-NH1	6.77	128.27	121.50
1	A	232	ASP	N-CA-C	6.68	120.72	111.90
1	A	226	ARG	CD-NE-CZ	6.61	133.66	124.40
1	A	340	TRP	CA-CB-CG	-6.19	101.84	113.60
1	A	210	LEU	N-CA-C	5.98	117.80	111.28
1	A	310	LEU	CB-CG-CD2	5.91	128.41	110.70
1	A	302	LEU	N-CA-CB	-5.62	101.86	110.01
1	A	272	ILE	N-CA-C	-5.52	102.46	109.58
1	A	325	PHE	CA-C-N	5.35	125.92	119.98
1	A	325	PHE	C-N-CA	5.35	125.92	119.98
1	A	363	GLU	N-CA-C	5.16	116.98	111.36
1	A	320	ASP	N-CA-C	-5.16	100.76	108.96
1	A	258	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	A	301	ARG	CB-CG-CD	5.03	122.88	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	ARG	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	1825	0	1882	24	2
2	B	55	0	62	0	0
3	A	16	0	27	0	0
4	A	77	0	0	2	0
All	All	1973	0	1971	24	2

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 (24) 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:A:265:LEU:HB3	1:A:266:PRO:HD3	1.74	0.69
1:A:267:PHE:CD1	1:A:272:ILE:HD12	2.29	0.66
1:A:321:SER:HB2	4:A:51:HOH:O	2.02	0.60
1:A:220:LEU:HD11	1:A:342:MET:SD	2.41	0.60
1:A:249:LEU:O	1:A:252:MET:HG2	2.07	0.55
1:A:310:LEU:O	1:A:314:ILE:HG12	2.08	0.53
1:A:267:PHE:CG	1:A:272:ILE:HD12	2.45	0.52
1:A:317:ARG:HD3	1:A:320:ASP:O	2.10	0.51
1:A:252:MET:CE	1:A:345:GLN:HB3	2.41	0.49
1:A:252:MET:HE3	1:A:345:GLN:HB3	1.95	0.48
1:A:265:LEU:HB3	1:A:266:PRO:CD	2.43	0.47
1:A:186:LEU:HD13	1:A:219:LEU:HD21	1.96	0.47
1:A:315:ASN:ND2	4:A:50:HOH:O	2.46	0.47
1:A:363:GLU:HA	1:A:368:GLY:HA2	1.96	0.47
1:A:314:ILE:O	1:A:317:ARG:HB2	2.15	0.46
1:A:208:VAL:CG1	1:A:212:ARG:HD3	2.49	0.42
1:A:314:ILE:HD12	1:A:324:ARG:HD3	2.01	0.42
1:A:345:GLN:O	1:A:349:ILE:HG12	2.19	0.42
1:A:350:LYS:HE2	1:A:362:GLN:OE1	2.20	0.42
1:A:192:TRP:CE2	1:A:281:LYS:HE3	2.55	0.42
1:A:352:PHE:CD1	1:A:352:PHE:N	2.87	0.42
1:A:252:MET:CE	1:A:349:ILE:HD11	2.49	0.42
1:A:212:ARG:NH1	1:A:363:GLU:O	2.53	0.41
1:A:221:LEU:HG	1:A:277:TYR:HE1	1.85	0.41

All (2) 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-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:CE3	1:A:340:TRP:CE3[5_655]	1.94	0.26
1:A:340:TRP:CE3	1:A:340:TRP:CZ3[5_655]	2.08	0.12

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	228/230 (99%)	218 (96%)	10 (4%)	0	100	100
2	B	7/9 (78%)	7 (100%)	0	0	100	100
All	All	235/239 (98%)	225 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	202/202 (100%)	192 (95%)	10 (5%)	22	28
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	205/205 (100%)	195 (95%)	10 (5%)	22	29

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	186	LEU
1	A	204	LEU
1	A	239	ASP
1	A	251	GLU
1	A	265	LEU
1	A	270	LEU
1	A	308	VAL
1	A	310	LEU
1	A	318	GLN

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

Mol	Chain	Res	Type
1	A	155	GLN

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Mol	Chain	Res	Type
1	A	271	GLN
1	A	315	ASN
1	A	318	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	MYR	A	500	-	15,15,15	1.68	1 (6%)	15,15,15	1.28	2 (13%)

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	MYR	A	500	-	-	7/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	MYR	O1-C1	5.91	1.41	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	MYR	O2-C1-O1	-3.02	115.58	123.33
3	A	500	MYR	C3-C2-C1	-2.27	108.60	114.51

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	MYR	C9-C10-C11-C12
3	A	500	MYR	C11-C10-C9-C8
3	A	500	MYR	C11-C12-C13-C14
3	A	500	MYR	C6-C7-C8-C9
3	A	500	MYR	C3-C4-C5-C6
3	A	500	MYR	C7-C8-C9-C10
3	A	500	MYR	C5-C6-C7-C8

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 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	230/230 (100%)	0.38	15 (6%)	25 22	19, 29, 64, 78	0
2	B	9/9 (100%)	2.69	6 (66%)	0 0	67, 72, 80, 81	0
All	All	239/239 (100%)	0.47	21 (8%)	15 13	19, 29, 71, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	6.2
2	B	8	ALA	5.0
1	A	368	GLY	4.1
1	A	163	ILE	4.1
2	B	11	ALA	3.8
1	A	159	PRO	3.2
2	B	16	ALA	3.1
1	A	319	TYR	2.9
1	A	340	TRP	2.9
1	A	320	ASP	2.8
1	A	160	VAL	2.8
2	B	15	ALA	2.7
2	B	9	ALA	2.7
1	A	164	ASN	2.6
1	A	248	GLU	2.4
1	A	348	PHE	2.4
1	A	139	SER	2.3
1	A	158	SER	2.3
1	A	141	PRO	2.2
1	A	295	ASP	2.1
2	B	14	LEU	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	MYR	A	500	16/16	0.88	0.14	18,30,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.