



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:17 AM GMT

PDB ID : 3A73
Title : Crystal Structure Analysis of Human serum albumin complexed with delta
12-prostaglandin J2
Authors : Ito, S.
Deposited on : 2009-09-11
Resolution : 2.19 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

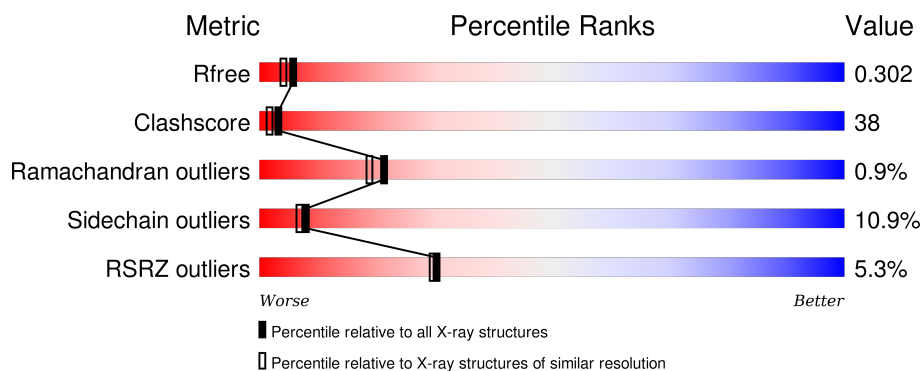
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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	585	<div> <div>5%</div> <div>57%</div> <div>35%</div> <div>5%</div> </div>
1	B	585	<div> <div>5%</div> <div>53%</div> <div>38%</div> <div>7%</div> </div>

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	MYR	A	1003	-	-	-	X
2	MYR	A	1004	-	-	X	-
2	MYR	A	1006	-	-	-	X
2	MYR	B	1002	-	-	-	X
2	MYR	B	1005	-	-	X	-
3	PJ2	A	1011	-	-	X	X
3	PJ2	A	1012	-	-	X	-
3	PJ2	B	1011	-	-	X	-

2 Entry composition [i](#)

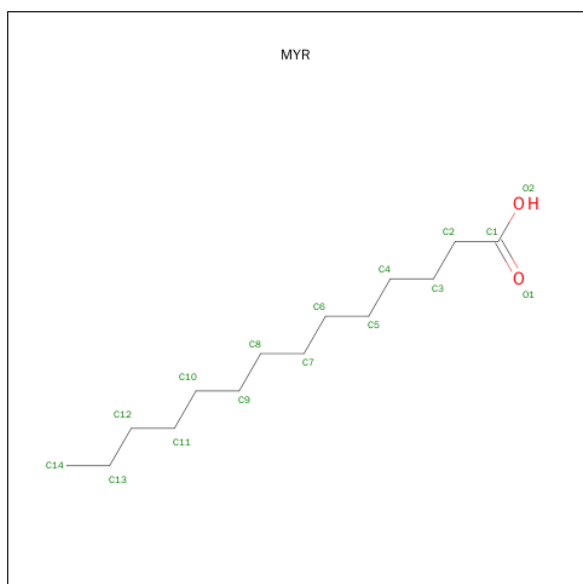
There are 4 unique types of molecules in this entry. The entry contains 9690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			
1	B	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C 12 12	0	0

- [illegible]

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 24	C 20	O 4	0	0
3	A	1	Total 24	C 20	O 4	0	0
3	B	1	Total 24	C 20	O 4	0	0

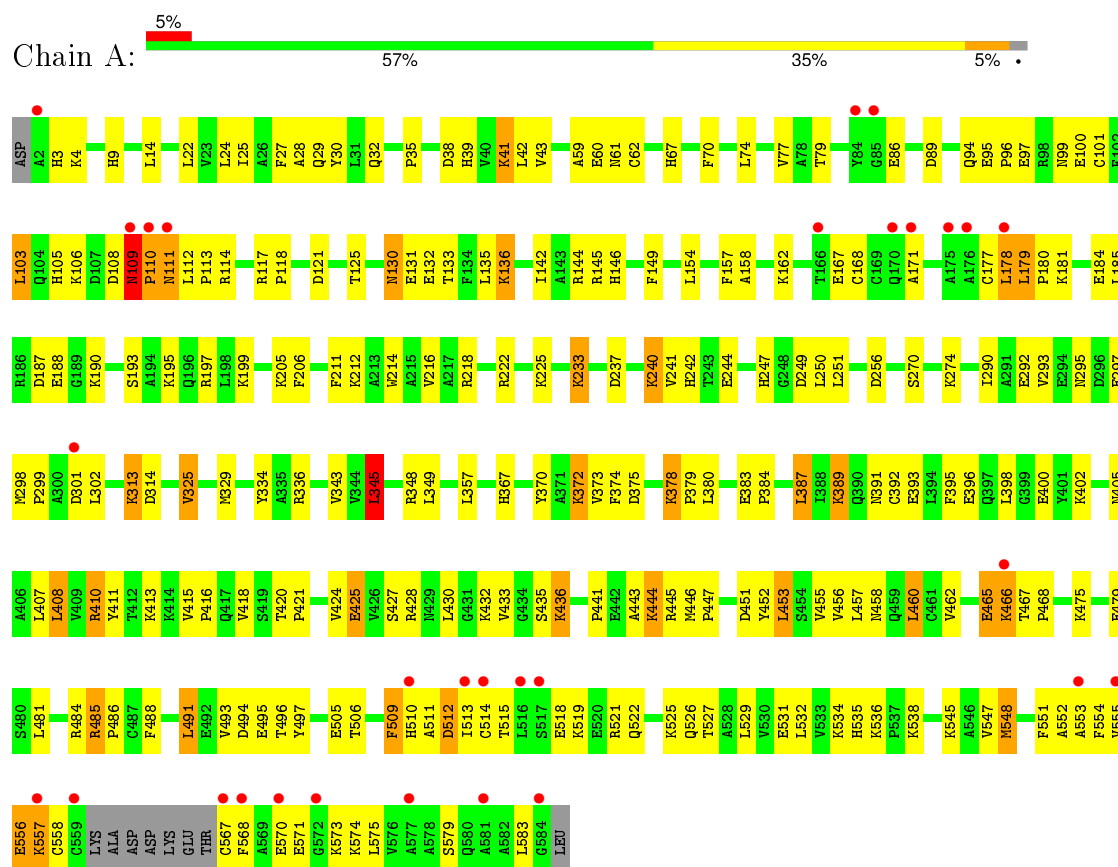
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	139	Total 139	O 139	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 ($\text{RSRZ} > 2$). 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: Serum albumin



Q522	E382	D451	E382	K262
I523	E383	T452	E383	
K524	P384	L453	P384	K274
K525	Q385	S454	Q385	L275
Q526	Q386	V455	N386	K276
	L387	V456		
E531		L457	E280	E280
L532		M458	K281	K281
V533		Q459	P282	P282
K534		L460	L283	L283
H535		C461	L284	L284
K536		V462	E285	E285
P537		E465	K286	K286
K538		K466	Q397	
A539		T467	L398	
T540		P468	Y401	T290
K541		V469	F403	A291
			K402	E294
K545			Q404	N295
A546			M405	D296
V547			A406	E297
H548			L407	M298
D549			L408	P299
P550			V409	
F551			R410	L302
A552				
A553			K413	S312
F554			K414	K313
V555			V415	D314
E556			P416	V315
K557			Q417	
C558			V418	Y334
C559			S419	
LYS			T420	R337
ALA			P421	
ASP			T422	Y341
ASP			L423	S342
LYS			V424	
GLU			E425	
THR			S427	L345
C567			R428	L347
F568			M429	R348
A569			L430	
E570				K351
E571				T352
G572			V433	Y353
K573			G434	
K574			S435	
L575				T356
V576			K439	L357
			H440	
Q580			P441	A371
A581				K372
A582				V373
L583			K444	F374
G584			R445	D375
LEU			M446	
			P447	
			C448	K378
			A449	P379
			E450	L380
				V381

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.06Å 92.05Å 94.66Å 74.80° 89.53° 80.21°	Depositor
Resolution (Å)	35.00 – 2.19 35.08 – 2.19	Depositor EDS
% Data completeness (in resolution range)	91.3 (35.00-2.19) 73.7 (35.08-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229 , 0.291 0.247 , 0.302	Depositor DCC
R_{free} test set	2871 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
Estimated twinning fraction	0.095 for h,h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57150 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: MYR, PJ2

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	0.91	1/4669 (0.0%)	0.91	4/6297 (0.1%)
1	B	0.89	4/4669 (0.1%)	0.88	3/6297 (0.0%)
All	All	0.90	5/9338 (0.1%)	0.89	7/12594 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	CB-CG2	5.47	1.64	1.52
1	B	371	ALA	CA-CB	5.46	1.64	1.52
1	B	348	ARG	C-N	-5.35	1.21	1.34
1	B	341	TYR	CD1-CE1	5.20	1.47	1.39
1	B	91	CYS	CB-SG	-5.18	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ALA	N-CA-C	5.90	126.94	111.00
1	A	336	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	171	ALA	N-CA-CB	-5.80	101.98	110.10
1	B	42	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	345	LEU	CB-CG-CD2	5.44	120.24	111.00

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	4580	0	4504	329	0
1	B	4580	0	4503	354	0
2	A	92	0	155	30	0
2	B	92	0	155	40	0
3	A	48	0	58	39	0
3	B	24	0	28	26	0
4	A	135	0	0	10	0
4	B	139	0	0	15	0
All	All	9690	0	9403	706	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 38.

The worst 5 of 706 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:146:HIS:CE1	3:A:1012:PJ2:HAI	1.39	1.57
1:A:146:HIS:CE1	3:A:1012:PJ2:CAI	2.01	1.40
1:A:142:ILE:CD1	3:A:1011:PJ2:HAAA	1.53	1.35
1:B:117:ARG:HD2	3:B:1011:PJ2:CAH	1.59	1.32
1:B:117:ARG:CG	3:B:1011:PJ2:HAH	1.61	1.30

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	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	21 19
1	B	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	21 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1144/1170 (98%)	1064 (93%)	70 (6%)	10 (1%)	21	19

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	PRO
1	B	94	GLN
1	A	111	ASN
1	B	95	GLU
1	A	479	GLU

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	503/511 (98%)	452 (90%)	51 (10%)	9	8
1	B	503/511 (98%)	444 (88%)	59 (12%)	7	5
All	All	1006/1022 (98%)	896 (89%)	110 (11%)	8	7

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	GLU
1	B	140	TYR
1	B	500	LYS
1	B	13	ASP
1	B	94	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	580	GLN
1	B	417	GLN

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Mol	Chain	Res	Type
1	A	440	HIS
1	A	522	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
2	MYR	A	1002	-	12,15,15	0.38	0	12,15,15	0.63	0
2	MYR	A	1003	-	12,15,15	0.74	0	12,15,15	1.03	1 (8%)
2	MYR	A	1004	-	12,15,15	0.30	0	12,15,15	1.53	2 (16%)
2	MYR	A	1005	-	12,15,15	0.35	0	12,15,15	0.90	0
2	MYR	A	1006	-	12,15,15	0.32	0	12,15,15	1.24	1 (8%)
2	MYR	A	1007	-	11,11,15	0.34	0	10,10,15	0.70	0
3	PJ2	A	1011	-	18,24,24	2.42	5 (27%)	20,29,29	2.70	5 (25%)
3	PJ2	A	1012	1	18,24,24	1.98	5 (27%)	20,29,29	1.56	2 (10%)
2	MYR	B	1002	-	12,15,15	0.48	0	12,15,15	0.56	0
2	MYR	B	1003	-	12,15,15	0.54	0	12,15,15	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYR	B	1004	-	12,15,15	0.39	0	12,15,15	1.31	2 (16%)
2	MYR	B	1005	-	12,15,15	0.46	0	12,15,15	0.48	0
2	MYR	B	1006	-	12,15,15	0.55	0	12,15,15	0.51	0
2	MYR	B	1007	-	11,11,15	0.27	0	10,10,15	0.75	0
3	PJ2	B	1011	-	18,24,24	2.21	8 (44%)	20,29,29	2.47	8 (40%)

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	MYR	A	1002	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1003	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1004	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1005	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1006	-	-	0/11/13/13	0/0/0/0
2	MYR	A	1007	-	-	0/9/9/13	0/0/0/0
3	PJ2	A	1011	-	-	0/17/32/32	0/1/1/1
3	PJ2	A	1012	1	-	0/17/32/32	0/1/1/1
2	MYR	B	1002	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1003	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1004	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1005	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1006	-	-	0/11/13/13	0/0/0/0
2	MYR	B	1007	-	-	0/9/9/13	0/0/0/0
3	PJ2	B	1011	-	-	0/17/32/32	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1011	PJ2	CAN-CAJ	-5.58	1.38	1.50
3	A	1012	PJ2	CAN-CAJ	-5.29	1.39	1.50
3	B	1011	PJ2	CAM-CAG	-4.80	1.34	1.50
3	B	1011	PJ2	CAN-CAJ	-4.39	1.41	1.50
3	A	1012	PJ2	CAM-CAG	-3.74	1.37	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1011	PJ2	OAC-CAU-CAV	-7.27	119.50	127.11
3	A	1011	PJ2	CAN-CAJ-CAV	-5.32	119.12	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1011	PJ2	OAC-CAU-CAV	-4.13	122.79	127.11
2	A	1004	MYR	C5-C4-C3	-3.42	96.89	114.53
2	B	1004	MYR	C4-C3-C2	-3.16	100.53	113.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	MYR	4	0
2	A	1003	MYR	4	0
2	A	1004	MYR	12	0
2	A	1005	MYR	6	0
2	A	1006	MYR	1	0
2	A	1007	MYR	3	0
3	A	1011	PJ2	22	0
3	A	1012	PJ2	22	0
2	B	1002	MYR	5	0
2	B	1003	MYR	8	0
2	B	1004	MYR	8	0
2	B	1005	MYR	11	0
2	B	1006	MYR	5	0
2	B	1007	MYR	3	0
3	B	1011	PJ2	26	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	576/585 (98%)	0.44	30 (5%) 31 30	19, 29, 37, 44	0
1	B	576/585 (98%)	0.50	31 (5%) 29 29	19, 30, 38, 44	0
All	All	1152/1170 (98%)	0.47	61 (5%) 30 29	19, 29, 37, 44	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	CYS	8.4
1	B	557	LYS	5.9
1	A	176	ALA	5.5
1	A	567	CYS	5.3
1	A	581	ALA	5.0

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 carbohydrates 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. 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
3	PJ2	A	1011	24/24	0.71	0.27	3.43	50,65,71,72	0
2	MYR	A	1006	16/16	0.76	0.21	2.83	44,53,59,60	0
2	MYR	A	1003	16/16	0.80	0.19	2.61	37,50,58,59	0
2	MYR	B	1002	16/16	0.82	0.18	2.25	40,49,56,56	0
3	PJ2	B	1011	24/24	0.73	0.20	1.81	46,61,65,65	0
2	MYR	B	1007	12/16	0.88	0.19	1.66	49,55,59,60	0
2	MYR	A	1002	16/16	0.85	0.17	1.51	37,48,62,62	0
2	MYR	B	1005	16/16	0.83	0.19	1.31	52,56,56,57	0
2	MYR	B	1003	16/16	0.89	0.14	0.66	33,40,47,48	0
2	MYR	B	1006	16/16	0.80	0.16	0.42	46,54,57,58	0
3	PJ2	A	1012	24/24	0.75	0.23	0.28	65,74,78,79	0
2	MYR	B	1004	16/16	0.89	0.15	0.14	45,49,53,55	0
2	MYR	A	1004	16/16	0.88	0.14	0.14	43,49,57,58	0
2	MYR	A	1005	16/16	0.88	0.16	0.04	43,48,57,59	0
2	MYR	A	1007	12/16	0.86	0.14	-0.15	52,53,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.