



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 AM GMT

PDB ID : 2OM9  
Title : Ajulemic acid, a synthetic cannabinoid bound to PPAR gamma  
Authors : Ambrosio, A.L.B.; Garratt, R.C.  
Deposited on : 2007-01-21  
Resolution : 2.80 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](mailto: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.

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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

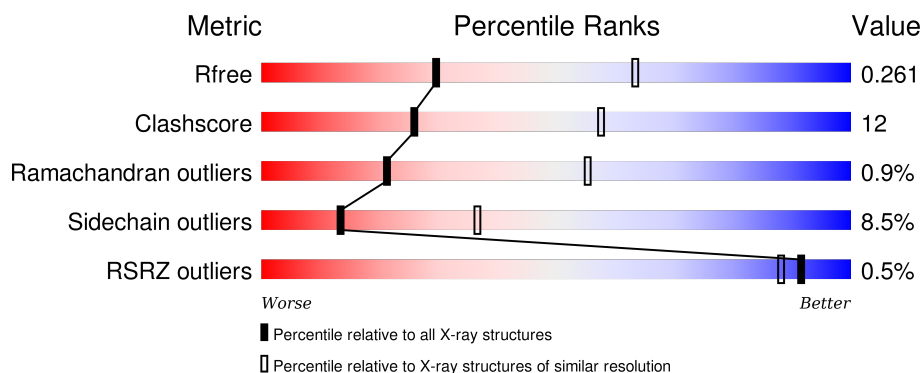
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	278	 74% 20% • • •
1	B	278	 68% 22% • 6%
1	C	278	 73% 22% • •
1	D	278	 66% 24% • 6%

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	AJA	B	601	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8965 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.

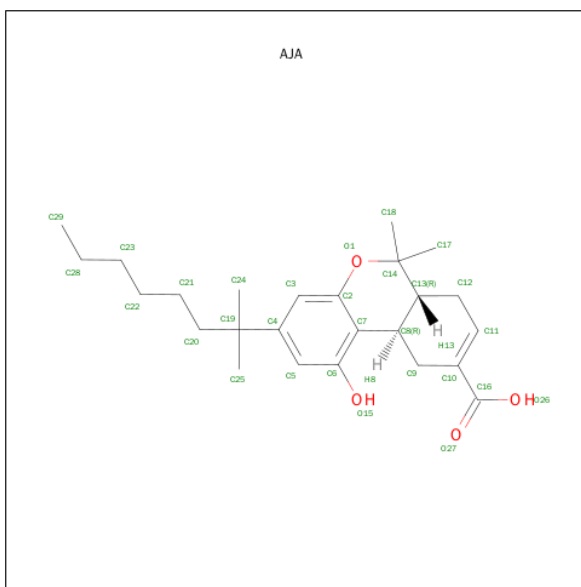
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	1	0
			2171	1401	354	406	10			
1	B	260	Total	C	N	O	S	0	0	0
			2089	1353	341	385	10			
1	C	270	Total	C	N	O	S	0	1	0
			2171	1401	354	406	10			
1	D	260	Total	C	N	O	S	0	0	0
			2089	1353	341	385	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	GLY	-	CLONING ARTIFACT	UNP P37231
A	201	SER	-	CLONING ARTIFACT	UNP P37231
A	202	HIS	-	CLONING ARTIFACT	UNP P37231
A	203	MET	-	CLONING ARTIFACT	UNP P37231
A	200	GLY	-	CLONING ARTIFACT	UNP P37231
A	201	SER	-	CLONING ARTIFACT	UNP P37231
A	202	HIS	-	CLONING ARTIFACT	UNP P37231
A	203	MET	-	CLONING ARTIFACT	UNP P37231
A	200	GLY	-	CLONING ARTIFACT	UNP P37231
A	201	SER	-	CLONING ARTIFACT	UNP P37231
A	202	HIS	-	CLONING ARTIFACT	UNP P37231
A	203	MET	-	CLONING ARTIFACT	UNP P37231
A	200	GLY	-	CLONING ARTIFACT	UNP P37231
A	201	SER	-	CLONING ARTIFACT	UNP P37231
A	202	HIS	-	CLONING ARTIFACT	UNP P37231
A	203	MET	-	CLONING ARTIFACT	UNP P37231

- Molecule 2 is (6AR,10AR)-3-(1,1-DIMETHYLHEPTYL)-1-HYDROXY-6,6-DIMETHYL-6A,7,10,10A-TETRAHYDRO-6H-BENZO[C]CHROMENE-9-CARBOXYLIC ACID (three-letter code: AJA) (formula: C<sub>25</sub>H<sub>36</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 29 25 4	0	0
2	B	1	Total C O 29 25 4	0	0
2	B	1	Total C O 29 25 4	0	0
2	A	1	Total C O 29 25 4	0	0
2	C	1	Total C O 29 25 4	0	0
2	C	1	Total C O 29 25 4	0	0
2	D	1	Total C O 29 25 4	0	0
2	D	1	Total C O 29 25 4	0	0

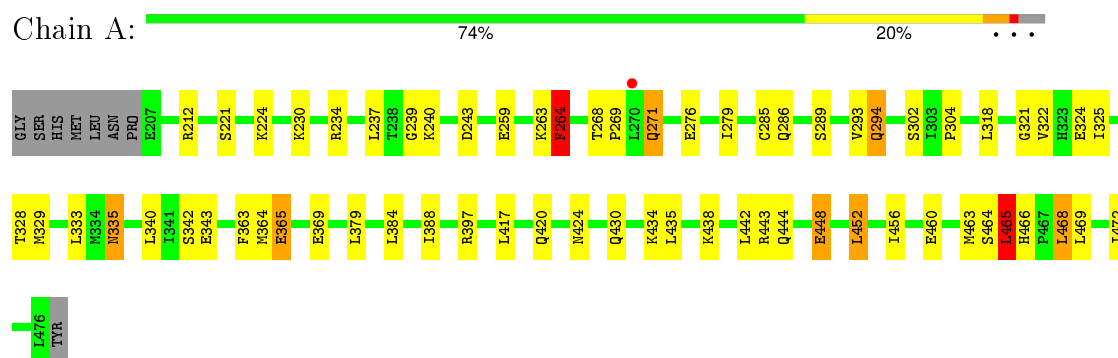
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0
3	B	46	Total O 46 46	0	0
3	C	61	Total O 61 61	0	0
3	D	41	Total O 41 41	0	0

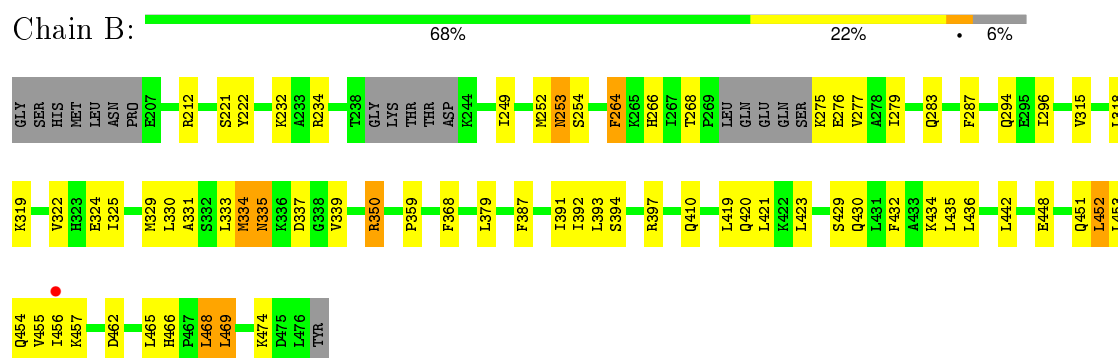
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

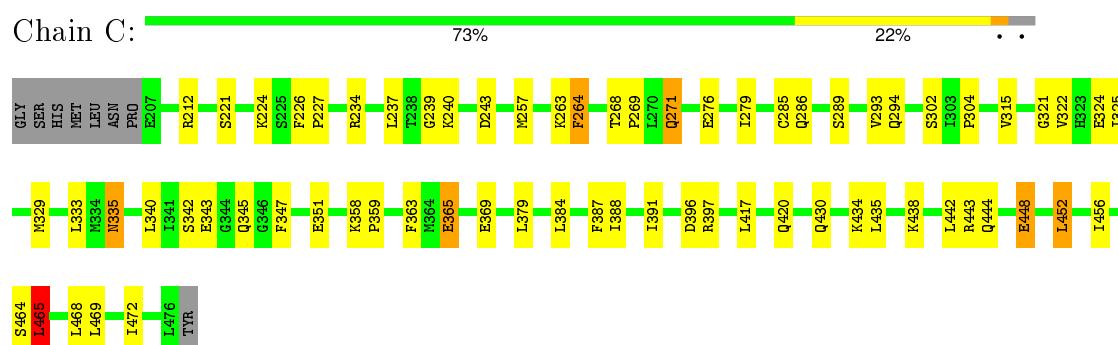
- Molecule 1: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma

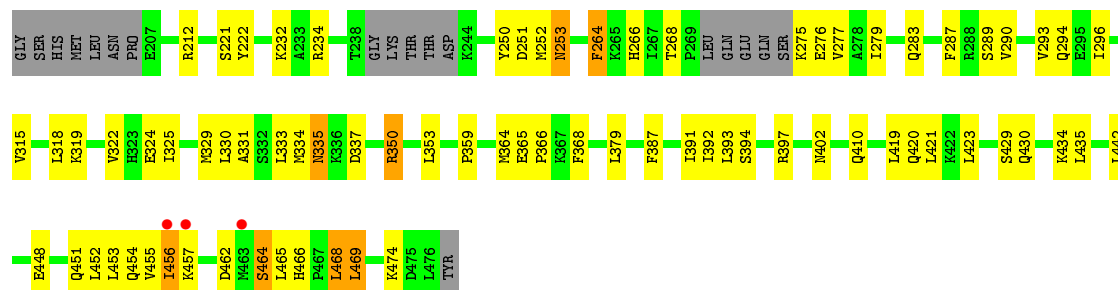


- Molecule 1: Peroxisome proliferator-activated receptor gamma



● Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.34Å 78.14Å 104.23Å 100.10° 106.41° 90.01°	Depositor
Resolution (Å)	10.00 – 2.80 29.12 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.8 (10.00-2.80) 84.1 (29.12-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.217 , 0.267 0.218 , 0.261	Depositor DCC
$R_{free}$ test set	2128 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 12.4	EDS
Estimated twinning fraction	0.297 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42977 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8965	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AJA

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	0.53	0/2211	0.65	0/2979
1	B	0.49	0/2124	0.61	0/2859
1	C	0.54	0/2211	0.66	0/2979
1	D	0.49	0/2124	0.61	0/2859
All	All	0.51	0/8670	0.64	0/11676

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	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	GLY	Peptide
1	A	264	PHE	Peptide
1	C	239	GLY	Peptide

## 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	2171	0	2238	49	0
1	B	2089	0	2158	53	0
1	C	2171	0	2238	41	0
1	D	2089	0	2158	51	0
2	A	58	0	68	14	0
2	B	58	0	68	11	0
2	C	58	0	68	12	0
2	D	58	0	68	10	0
3	A	65	0	0	3	0
3	B	46	0	0	2	0
3	C	61	0	0	2	0
3	D	41	0	0	3	0
All	All	8965	0	9064	218	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 12.

All (218) 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:D:264:PHE:CD2	2:D:802:AJA:H11	1.90	1.06
1:A:264:PHE:HB2	2:A:501:AJA:O26	1.76	0.86
1:D:264:PHE:CG	2:D:802:AJA:H11	2.11	0.84
1:C:264:PHE:CD2	2:C:701:AJA:H11	2.12	0.84
1:C:384:LEU:O	1:C:388:ILE:HG12	1.79	0.83
2:C:701:AJA:H92	2:C:701:AJA:O15	1.81	0.80
2:D:802:AJA:O15	2:D:802:AJA:H92	1.81	0.79
1:B:330:LEU:O	1:B:334:MET:HG2	1.84	0.78
1:D:379:LEU:HD11	1:D:435:LEU:HD11	1.66	0.75
1:B:379:LEU:HD11	1:B:435:LEU:HD11	1.69	0.74
1:C:264:PHE:CG	2:C:701:AJA:H11	2.21	0.74
1:B:468:LEU:HA	2:B:502:AJA:H243	1.69	0.73
1:D:330:LEU:O	1:D:334:MET:HG2	1.88	0.73
1:B:430:GLN:O	1:B:434:LYS:HG3	1.89	0.73
1:A:286:GLN:HE22	1:A:465:LEU:HD23	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HB2	2:A:501:AJA:C16	2.18	0.71
1:A:384:LEU:O	1:A:388:ILE:HG12	1.90	0.70
1:A:430:GLN:O	1:A:434:LYS:HG3	1.91	0.70
1:D:430:GLN:O	1:D:434:LYS:HG3	1.92	0.70
1:D:359:PRO:HG2	1:D:456:ILE:HD13	1.74	0.70
1:A:212:ARG:HH12	1:A:420:GLN:HE21	1.39	0.69
1:D:264:PHE:CD2	2:D:802:AJA:C11	2.73	0.69
1:C:286:GLN:HE22	1:C:465:LEU:HD23	1.57	0.69
1:D:212:ARG:HH12	1:D:420:GLN:HE21	1.41	0.69
1:C:302:SER:HB3	3:C:735:HOH:O	1.93	0.68
1:A:466:HIS:CD2	1:A:468:LEU:H	2.11	0.68
1:A:466:HIS:HD2	1:A:468:LEU:H	1.39	0.68
1:B:212:ARG:HH12	1:B:420:GLN:HE21	1.41	0.68
1:A:466:HIS:HE1	3:A:65:HOH:O	1.76	0.68
1:B:264:PHE:HB2	2:B:601:AJA:O26	1.94	0.67
1:D:464:SER:HB2	3:D:839:HOH:O	1.95	0.66
2:C:701:AJA:C9	2:C:701:AJA:O15	2.44	0.66
2:C:702:AJA:H92	2:C:702:AJA:O15	1.96	0.66
2:D:802:AJA:O15	2:D:802:AJA:C9	2.44	0.65
2:B:502:AJA:H92	2:B:502:AJA:O15	1.97	0.65
1:C:430:GLN:O	1:C:434:LYS:HG3	1.96	0.65
1:B:275:LYS:HE2	1:B:462:ASP:HB2	1.78	0.65
2:B:601:AJA:O15	2:B:601:AJA:H92	1.96	0.65
2:A:501:AJA:H92	2:A:501:AJA:O15	1.95	0.64
1:A:318:LEU:HB3	2:B:502:AJA:H291	1.78	0.64
2:D:801:AJA:O15	2:D:801:AJA:H92	1.96	0.64
2:C:701:AJA:H211	2:C:701:AJA:C3	2.27	0.64
2:B:502:AJA:C9	2:B:502:AJA:O15	2.46	0.64
1:A:468:LEU:HA	2:A:602:AJA:H252	1.79	0.64
1:C:269:PRO:HB2	1:C:271:GLN:OE1	1.98	0.64
2:A:602:AJA:H92	2:A:602:AJA:O15	1.96	0.64
2:C:702:AJA:O15	2:C:702:AJA:C9	2.46	0.63
1:D:252:MET:SD	1:D:277:VAL:HG11	2.39	0.63
2:A:602:AJA:O15	2:A:602:AJA:C9	2.46	0.63
1:A:466:HIS:CE1	2:A:602:AJA:H172	2.33	0.63
1:B:279:ILE:O	1:B:283:GLN:HG2	1.98	0.63
2:A:501:AJA:C9	2:A:501:AJA:O15	2.46	0.63
2:B:601:AJA:O15	2:B:601:AJA:C9	2.47	0.63
2:D:801:AJA:O15	2:D:801:AJA:C9	2.46	0.62
1:C:276:GLU:HG2	1:C:279:ILE:HD12	1.81	0.62
1:D:275:LYS:HE2	1:D:462:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:HD11	1:D:392:ILE:HG13	1.81	0.62
1:A:468:LEU:HD23	2:A:602:AJA:H252	1.82	0.61
2:A:602:AJA:H222	1:B:315:VAL:HG13	1.82	0.61
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.81	0.61
1:B:419:LEU:CD1	1:B:423:LEU:HD21	2.30	0.61
1:C:379:LEU:HD11	1:C:435:LEU:HD11	1.83	0.61
1:C:321:GLY:O	1:C:325:ILE:HG12	2.01	0.61
1:B:335:ASN:HD22	1:B:337:ASP:H	1.46	0.60
1:A:269:PRO:HB2	1:A:271:GLN:OE1	2.02	0.60
1:C:263:LYS:HB3	1:C:345:GLN:HE22	1.66	0.60
1:D:279:ILE:O	1:D:283:GLN:HG2	2.01	0.59
1:D:212:ARG:HH12	1:D:420:GLN:NE2	2.00	0.59
1:D:315:VAL:HG13	2:D:801:AJA:H222	1.85	0.59
1:D:387:PHE:CE2	1:D:391:ILE:HD11	2.38	0.58
1:D:335:ASN:HD22	1:D:337:ASP:H	1.49	0.58
1:B:350:ARG:HD3	1:B:368:PHE:CG	2.39	0.58
1:B:212:ARG:HH12	1:B:420:GLN:NE2	2.00	0.58
1:A:276:GLU:HG2	1:A:279:ILE:HD12	1.86	0.57
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.70	0.57
1:A:230:LYS:NZ	1:A:379:LEU:O	2.25	0.57
1:B:335:ASN:ND2	1:B:337:ASP:H	2.03	0.57
1:D:335:ASN:ND2	1:D:337:ASP:H	2.03	0.57
2:D:802:AJA:C3	2:D:802:AJA:H211	2.36	0.56
1:A:468:LEU:HD23	2:A:602:AJA:C25	2.35	0.56
1:C:212:ARG:HH12	1:C:420:GLN:HE21	1.52	0.56
1:B:359:PRO:HG2	1:B:456:ILE:HD13	1.86	0.56
1:B:329:MET:HG3	3:B:104:HOH:O	2.04	0.56
1:A:329:MET:HE2	3:A:81:HOH:O	2.05	0.56
1:D:419:LEU:CD1	1:D:423:LEU:HD21	2.36	0.55
1:B:252:MET:SD	1:B:277:VAL:HG11	2.46	0.55
2:C:702:AJA:H221	2:C:702:AJA:C4	2.36	0.55
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.88	0.55
1:B:429:SER:O	1:B:430:GLN:HB2	2.06	0.55
1:A:212:ARG:HH22	1:A:420:GLN:HE22	1.55	0.55
1:D:350:ARG:HD3	1:D:368:PHE:CG	2.42	0.54
1:B:393:LEU:O	1:B:410:GLN:HB2	2.08	0.54
1:D:419:LEU:O	1:D:423:LEU:HD23	2.07	0.53
1:C:363:PHE:HE2	1:C:456:ILE:HD11	1.74	0.53
1:D:325:ILE:HD11	1:D:392:ILE:CG1	2.38	0.53
1:D:429:SER:O	1:D:430:GLN:HB2	2.08	0.53
1:C:315:VAL:HG13	2:C:702:AJA:H222	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:SER:O	1:C:304:PRO:HD3	2.09	0.53
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.39	0.52
1:A:294:GLN:OE1	1:B:294:GLN:NE2	2.42	0.52
1:C:325:ILE:HD12	1:C:388:ILE:HG23	1.92	0.52
1:D:453:LEU:C	1:D:455:VAL:H	2.12	0.52
1:B:419:LEU:HD11	1:B:423:LEU:HD21	1.91	0.51
1:B:453:LEU:C	1:B:455:VAL:H	2.13	0.51
1:B:394:SER:O	1:B:397:ARG:HG2	2.11	0.51
1:C:464:SER:O	1:C:465:LEU:C	2.48	0.51
1:A:379:LEU:HD11	1:A:435:LEU:HD11	1.93	0.51
1:D:359:PRO:HG2	1:D:456:ILE:CD1	2.39	0.51
1:A:259:GLU:HA	1:A:264:PHE:CZ	2.46	0.50
1:B:276:GLU:HG3	1:B:279:ILE:HG12	1.93	0.50
1:C:322:VAL:HG21	1:C:472:ILE:HD13	1.92	0.50
1:A:328:THR:HG21	1:A:388:ILE:HD11	1.93	0.50
1:C:212:ARG:HH22	1:C:420:GLN:HE22	1.60	0.50
1:A:464:SER:O	1:A:465:LEU:C	2.49	0.50
1:B:419:LEU:O	1:B:423:LEU:HD23	2.11	0.50
1:D:392:ILE:HG22	1:D:393:LEU:HD22	1.92	0.50
1:B:452:LEU:HD12	3:B:26:HOH:O	2.11	0.50
1:A:365:GLU:OE1	1:A:365:GLU:HA	2.12	0.49
1:B:212:ARG:HH22	1:B:420:GLN:HE22	1.60	0.49
1:A:452:LEU:O	1:A:456:ILE:HG12	2.13	0.49
1:A:302:SER:O	1:A:304:PRO:HD3	2.13	0.48
1:D:393:LEU:O	1:D:410:GLN:HB2	2.14	0.48
1:D:324:GLU:HG2	1:D:442:LEU:HB3	1.95	0.48
1:B:466:HIS:HB3	1:B:469:LEU:HD22	1.95	0.48
1:A:289:SER:O	1:A:293:VAL:HG23	2.14	0.48
1:A:263:LYS:HG2	1:A:263:LYS:O	2.13	0.47
1:B:387:PHE:CE2	1:B:391:ILE:HD11	2.50	0.47
1:C:434:LYS:O	1:C:438:LYS:HG2	2.15	0.47
1:C:417:LEU:HD21	1:C:435:LEU:HD23	1.96	0.47
1:C:324:GLU:OE2	1:C:397:ARG:NH1	2.36	0.47
1:C:324:GLU:OE2	1:C:443:ARG:HG3	2.14	0.47
1:D:253:ASN:H	1:D:253:ASN:ND2	2.12	0.47
1:B:331:ALA:HA	1:B:334:MET:HG3	1.96	0.47
1:B:419:LEU:O	1:B:423:LEU:CD2	2.63	0.46
1:D:419:LEU:O	1:D:423:LEU:CD2	2.64	0.46
1:D:276:GLU:HG3	1:D:279:ILE:HG12	1.97	0.46
1:D:335:ASN:C	1:D:335:ASN:HD22	2.18	0.46
1:B:324:GLU:HG2	1:B:442:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:LEU:HD11	1:D:423:LEU:HD21	1.96	0.46
1:C:452:LEU:O	1:C:456:ILE:HG12	2.15	0.46
1:C:387:PHE:CE2	1:C:391:ILE:HD11	2.51	0.46
1:D:331:ALA:HA	1:D:334:MET:HG3	1.98	0.46
1:B:334:MET:HE3	1:B:339:VAL:HG21	1.97	0.46
1:A:212:ARG:HH12	1:A:420:GLN:NE2	2.10	0.46
2:B:502:AJA:H253	2:B:502:AJA:H212	1.55	0.46
1:D:466:HIS:HB3	1:D:469:LEU:HD22	1.97	0.45
1:C:335:ASN:C	1:C:335:ASN:HD22	2.19	0.45
1:A:444:GLN:NE2	1:A:448:GLU:OE2	2.50	0.45
1:A:321:GLY:O	1:A:325:ILE:HG12	2.17	0.45
1:D:394:SER:O	1:D:397:ARG:HG2	2.17	0.45
1:D:325:ILE:O	1:D:329:MET:HG2	2.17	0.45
1:C:329:MET:HE2	3:C:726:HOH:O	2.16	0.45
1:A:434:LYS:O	1:A:438:LYS:HG2	2.17	0.45
1:B:419:LEU:HD12	1:B:423:LEU:CD2	2.47	0.45
2:D:802:AJA:H211	2:D:802:AJA:H3	1.98	0.45
1:B:335:ASN:HD22	1:B:335:ASN:C	2.20	0.45
1:C:335:ASN:HD22	1:C:335:ASN:H	1.65	0.44
1:B:350:ARG:HB2	1:B:368:PHE:CZ	2.52	0.44
1:A:466:HIS:HD2	1:A:468:LEU:N	2.13	0.44
2:A:602:AJA:H121	3:A:65:HOH:O	2.17	0.44
1:B:392:ILE:HG22	1:B:393:LEU:HD22	1.98	0.44
1:D:253:ASN:N	1:D:253:ASN:ND2	2.65	0.44
1:B:466:HIS:CE1	2:B:502:AJA:H172	2.53	0.44
2:A:602:AJA:H211	2:A:602:AJA:H242	1.69	0.44
1:D:252:MET:CE	1:D:277:VAL:HG21	2.47	0.44
1:C:358:LYS:HA	1:C:359:PRO:HA	1.70	0.44
1:C:264:PHE:CD2	2:C:701:AJA:C11	2.95	0.44
1:A:417:LEU:HD21	1:A:435:LEU:HD23	1.99	0.44
1:B:432:PHE:O	1:B:436:LEU:HG	2.17	0.43
1:D:250:TYR:CE2	1:D:251:ASP:OD1	2.71	0.43
1:C:444:GLN:NE2	1:C:448:GLU:OE2	2.51	0.43
1:D:353:LEU:HD13	1:D:364:MET:HG3	2.01	0.43
1:A:237:LEU:HD21	1:A:340:LEU:HG	2.00	0.43
1:B:296:ILE:HG21	1:B:322:VAL:HG12	2.00	0.43
2:B:601:AJA:H253	2:B:601:AJA:H212	1.82	0.43
1:D:365:GLU:N	1:D:366:PRO:HD2	2.34	0.43
1:D:296:ILE:HG21	1:D:322:VAL:HG12	2.00	0.43
2:C:701:AJA:C21	2:C:701:AJA:C3	2.97	0.43
1:B:419:LEU:CD1	1:B:423:LEU:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:OE2	1:A:443:ARG:HG3	2.19	0.43
1:B:264:PHE:HB2	2:B:601:AJA:C16	2.48	0.42
1:B:325:ILE:O	1:B:329:MET:HG2	2.19	0.42
1:D:402:ASN:HB2	3:D:819:HOH:O	2.18	0.42
1:C:289:SER:O	1:C:293:VAL:HG23	2.18	0.42
1:A:335:ASN:C	1:A:335:ASN:HD22	2.22	0.42
1:B:252:MET:CE	1:B:277:VAL:HG21	2.49	0.42
1:B:212:ARG:HA	1:B:212:ARG:HD2	1.73	0.42
1:D:266:HIS:CE1	1:D:287:PHE:CE1	3.08	0.42
1:A:328:THR:HG21	1:A:388:ILE:CD1	2.50	0.42
1:C:396:ASP:CG	1:C:443:ARG:HH12	2.23	0.42
1:B:266:HIS:CE1	1:B:287:PHE:CE1	3.08	0.42
1:B:253:ASN:ND2	1:B:253:ASN:H	2.17	0.42
2:A:602:AJA:C4	2:A:602:AJA:H221	2.50	0.42
1:B:452:LEU:O	1:B:455:VAL:HB	2.20	0.42
1:D:402:ASN:HA	3:D:834:HOH:O	2.19	0.42
1:D:212:ARG:HA	1:D:212:ARG:HD2	1.73	0.41
1:A:324:GLU:OE2	1:A:397:ARG:NH1	2.39	0.41
1:D:421:LEU:HD11	1:D:435:LEU:HD22	2.02	0.41
1:A:424:ASN:O	1:C:351:GLU:HG2	2.19	0.41
1:B:421:LEU:HD11	1:B:435:LEU:HD22	2.01	0.41
1:D:290:VAL:HG13	1:D:468:LEU:HD12	2.03	0.41
1:C:237:LEU:HD21	1:C:340:LEU:HG	2.03	0.41
1:A:325:ILE:O	1:A:329:MET:HG3	2.21	0.41
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.89	0.41
1:C:285:CYS:SG	2:C:701:AJA:H222	2.61	0.41
1:D:350:ARG:HD2	1:D:365:GLU:OE1	2.21	0.41
1:A:364:MET:O	1:A:365:GLU:C	2.58	0.41
1:A:212:ARG:HH22	1:A:420:GLN:NE2	2.17	0.41
1:D:289:SER:O	1:D:293:VAL:HG23	2.20	0.41
1:C:226:PHE:HA	1:C:227:PRO:HD2	1.91	0.41
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.89	0.41
1:C:325:ILE:O	1:C:329:MET:HG3	2.21	0.40
1:C:365:GLU:OE1	1:C:365:GLU:HA	2.20	0.40
1:A:318:LEU:O	1:A:322:VAL:HG13	2.21	0.40
1:C:335:ASN:HD21	1:C:347:PHE:HZ	1.68	0.40
1:B:253:ASN:N	1:B:253:ASN:ND2	2.69	0.40
1:A:460:GLU:HB3	1:A:463:MET:HE2	2.03	0.40
1:B:249:ILE:HA	1:B:254:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	269/278 (97%)	254 (94%)	13 (5%)	2 (1%)	26	62
1	B	254/278 (91%)	234 (92%)	18 (7%)	2 (1%)	24	58
1	C	269/278 (97%)	254 (94%)	13 (5%)	2 (1%)	26	62
1	D	254/278 (91%)	236 (93%)	15 (6%)	3 (1%)	16	47
All	All	1046/1112 (94%)	978 (94%)	59 (6%)	9 (1%)	21	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	465	LEU
1	C	243	ASP
1	C	465	LEU
1	B	454	GLN
1	D	454	GLN
1	D	474	LYS
1	B	474	LYS
1	D	456	ILE

### 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	244/250 (98%)	223 (91%)	21 (9%)	13	36
1	B	234/250 (94%)	214 (92%)	20 (8%)	13	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	244/250 (98%)	223 (91%)	21 (9%)	13	36
1	D	234/250 (94%)	213 (91%)	21 (9%)	12	34
All	All	956/1000 (96%)	873 (91%)	83 (9%)	13	35

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	224	LYS
1	A	234	ARG
1	A	240	LYS
1	A	264	PHE
1	A	268	THR
1	A	271	GLN
1	A	285	CYS
1	A	294	GLN
1	A	333	LEU
1	A	335	ASN
1	A	342	SER
1	A	343[A]	GLU
1	A	343[B]	GLU
1	A	365	GLU
1	A	369	GLU
1	A	448	GLU
1	A	452	LEU
1	A	465	LEU
1	A	468	LEU
1	A	469	LEU
1	B	221	SER
1	B	222	TYR
1	B	232	LYS
1	B	234	ARG
1	B	253	ASN
1	B	264	PHE
1	B	268	THR
1	B	318	LEU
1	B	319	LYS
1	B	333	LEU
1	B	334	MET
1	B	335	ASN
1	B	350	ARG

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Mol	Chain	Res	Type
1	B	448	GLU
1	B	451	GLN
1	B	452	LEU
1	B	457	LYS
1	B	465	LEU
1	B	468	LEU
1	B	469	LEU
1	C	221	SER
1	C	224	LYS
1	C	234	ARG
1	C	240	LYS
1	C	257	MET
1	C	264	PHE
1	C	268	THR
1	C	271	GLN
1	C	294	GLN
1	C	333	LEU
1	C	335	ASN
1	C	342	SER
1	C	343[A]	GLU
1	C	343[B]	GLU
1	C	365	GLU
1	C	369	GLU
1	C	448	GLU
1	C	452	LEU
1	C	465	LEU
1	C	468	LEU
1	C	469	LEU
1	D	221	SER
1	D	222	TYR
1	D	232	LYS
1	D	234	ARG
1	D	253	ASN
1	D	264	PHE
1	D	268	THR
1	D	294	GLN
1	D	318	LEU
1	D	319	LYS
1	D	333	LEU
1	D	335	ASN
1	D	350	ARG
1	D	448	GLU

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Mol	Chain	Res	Type
1	D	451	GLN
1	D	452	LEU
1	D	457	LYS
1	D	464	SER
1	D	465	LEU
1	D	468	LEU
1	D	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	273	GLN
1	A	286	GLN
1	A	335	ASN
1	A	345	GLN
1	A	410	GLN
1	A	412	ASN
1	A	420	GLN
1	A	466	HIS
1	B	253	ASN
1	B	283	GLN
1	B	308	ASN
1	B	335	ASN
1	B	412	ASN
1	B	420	GLN
1	B	466	HIS
1	C	273	GLN
1	C	335	ASN
1	C	345	GLN
1	C	410	GLN
1	C	412	ASN
1	C	420	GLN
1	D	253	ASN
1	D	266	HIS
1	D	283	GLN
1	D	335	ASN
1	D	412	ASN
1	D	420	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	AJA	A	501	-	29,31,31	0.96	4 (13%)	37,47,47	1.30	3 (8%)
2	AJA	A	602	-	29,31,31	0.96	4 (13%)	37,47,47	1.29	3 (8%)
2	AJA	B	502	-	29,31,31	0.96	4 (13%)	37,47,47	1.30	3 (8%)
2	AJA	B	601	-	29,31,31	0.96	4 (13%)	37,47,47	1.30	3 (8%)
2	AJA	C	701	-	29,31,31	0.96	3 (10%)	37,47,47	1.33	2 (5%)
2	AJA	C	702	-	29,31,31	0.96	4 (13%)	37,47,47	1.30	3 (8%)
2	AJA	D	801	-	29,31,31	0.95	4 (13%)	37,47,47	1.30	3 (8%)
2	AJA	D	802	-	29,31,31	0.97	4 (13%)	37,47,47	1.32	2 (5%)

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	AJA	A	501	-	-	0/13/45/45	0/3/3/3
2	AJA	A	602	-	-	0/13/45/45	0/3/3/3
2	AJA	B	502	-	-	0/13/45/45	0/3/3/3
2	AJA	B	601	-	-	0/13/45/45	0/3/3/3
2	AJA	C	701	-	-	0/13/45/45	0/3/3/3
2	AJA	C	702	-	-	0/13/45/45	0/3/3/3
2	AJA	D	801	-	-	0/13/45/45	0/3/3/3
2	AJA	D	802	-	-	0/13/45/45	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	AJA	C16-C10	-2.87	1.46	1.51
2	D	802	AJA	C16-C10	-2.86	1.46	1.51
2	C	702	AJA	C16-C10	-2.85	1.46	1.51
2	B	601	AJA	C16-C10	-2.85	1.46	1.51
2	A	602	AJA	C16-C10	-2.84	1.46	1.51
2	A	501	AJA	C16-C10	-2.82	1.46	1.51
2	D	801	AJA	C16-C10	-2.82	1.46	1.51
2	C	701	AJA	C16-C10	-2.79	1.46	1.51
2	C	701	AJA	C7-C8	-2.27	1.48	1.51
2	D	802	AJA	C7-C8	-2.26	1.48	1.51
2	A	602	AJA	C7-C8	-2.19	1.48	1.51
2	D	801	AJA	C7-C8	-2.19	1.48	1.51
2	A	501	AJA	C7-C8	-2.19	1.48	1.51
2	B	502	AJA	C7-C8	-2.13	1.48	1.51
2	B	502	AJA	C19-C4	-2.13	1.50	1.53
2	A	602	AJA	O1-C14	-2.13	1.42	1.47
2	C	702	AJA	C7-C8	-2.13	1.48	1.51
2	B	601	AJA	C7-C8	-2.12	1.48	1.51
2	A	501	AJA	C19-C4	-2.10	1.50	1.53
2	C	701	AJA	C19-C4	-2.10	1.50	1.53
2	B	601	AJA	C19-C4	-2.10	1.50	1.53
2	A	602	AJA	C19-C4	-2.09	1.50	1.53
2	C	702	AJA	O1-C14	-2.09	1.42	1.47
2	B	502	AJA	O1-C14	-2.08	1.42	1.47
2	D	801	AJA	O1-C14	-2.07	1.42	1.47
2	C	702	AJA	C19-C4	-2.06	1.50	1.53
2	D	802	AJA	C19-C4	-2.06	1.50	1.53
2	B	601	AJA	O1-C14	-2.06	1.43	1.47
2	A	501	AJA	O1-C14	-2.05	1.43	1.47
2	D	801	AJA	C19-C4	-2.05	1.50	1.53
2	D	802	AJA	O1-C14	-2.01	1.43	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	AJA	C8-C9-C10	-5.04	109.25	113.08
2	D	802	AJA	C8-C9-C10	-4.98	109.29	113.08
2	A	501	AJA	C8-C9-C10	-4.80	109.42	113.08
2	D	801	AJA	C8-C9-C10	-4.77	109.45	113.08
2	B	601	AJA	C8-C9-C10	-4.75	109.46	113.08
2	C	702	AJA	C8-C9-C10	-4.72	109.48	113.08
2	B	502	AJA	C8-C9-C10	-4.72	109.49	113.08
2	A	602	AJA	C8-C9-C10	-4.70	109.50	113.08
2	C	702	AJA	C21-C20-C19	-3.01	110.96	117.11
2	A	602	AJA	C21-C20-C19	-3.01	110.97	117.11
2	A	501	AJA	C21-C20-C19	-3.00	110.99	117.11
2	D	801	AJA	C21-C20-C19	-3.00	111.00	117.11
2	B	601	AJA	C21-C20-C19	-2.99	111.00	117.11
2	D	802	AJA	C21-C20-C19	-2.99	111.01	117.11
2	C	701	AJA	C21-C20-C19	-2.98	111.02	117.11
2	B	502	AJA	C21-C20-C19	-2.98	111.04	117.11
2	A	501	AJA	C9-C8-C7	-2.07	109.31	113.24
2	B	502	AJA	C9-C8-C7	-2.06	109.34	113.24
2	D	801	AJA	C9-C8-C7	-2.05	109.34	113.24
2	C	702	AJA	C9-C8-C7	-2.04	109.38	113.24
2	B	601	AJA	C9-C8-C7	-2.04	109.38	113.24
2	A	602	AJA	C9-C8-C7	-2.03	109.39	113.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AJA	4	0
2	A	602	AJA	10	0
2	B	502	AJA	6	0
2	B	601	AJA	5	0
2	C	701	AJA	8	0
2	C	702	AJA	4	0
2	D	801	AJA	3	0
2	D	802	AJA	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	270/278 (97%)	-0.20	1 (0%) 93 90	18, 32, 56, 70	6 (2%)
1	B	260/278 (93%)	-0.14	1 (0%) 93 90	19, 41, 76, 81	7 (2%)
1	C	270/278 (97%)	-0.20	0 100 100	19, 32, 55, 70	6 (2%)
1	D	260/278 (93%)	-0.18	3 (1%) 81 73	19, 40, 75, 82	7 (2%)
All	All	1060/1112 (95%)	-0.18	5 (0%) 91 88	18, 36, 69, 82	26 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	ILE	2.6
1	A	270	LEU	2.4
1	D	463	MET	2.3
1	D	457	LYS	2.2
1	D	456	ILE	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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	AJA	B	601	29/29	0.88	0.40	3.02	43,45,46,47	0
2	AJA	D	801	29/29	0.93	0.23	1.88	25,27,32,33	0
2	AJA	C	702	29/29	0.91	0.24	1.57	28,29,34,35	0
2	AJA	A	602	29/29	0.95	0.23	1.42	22,29,33,36	0
2	AJA	D	802	29/29	0.91	0.29	1.08	37,42,46,47	0
2	AJA	B	502	29/29	0.92	0.22	0.81	28,29,33,37	0
2	AJA	C	701	29/29	0.95	0.22	0.66	30,33,37,39	0
2	AJA	A	501	29/29	0.93	0.21	0.09	21,27,30,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.