



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:18 AM GMT

PDB ID : 2Q60  
Title : Crystal structure of the ligand binding domain of polyandrocarpa misakiensis rxr in tetramer in absence of ligand  
Authors : Borel, F.; De Groot, A.; Juillan-Binard, C.; De Rosny, E.; Laudet, V.; Pebay-Peyroula, E.; Fontecilla-Camps, J.-C.; Ferrer, J.-L.  
Deposited on : 2007-06-04  
Resolution : 2.90 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

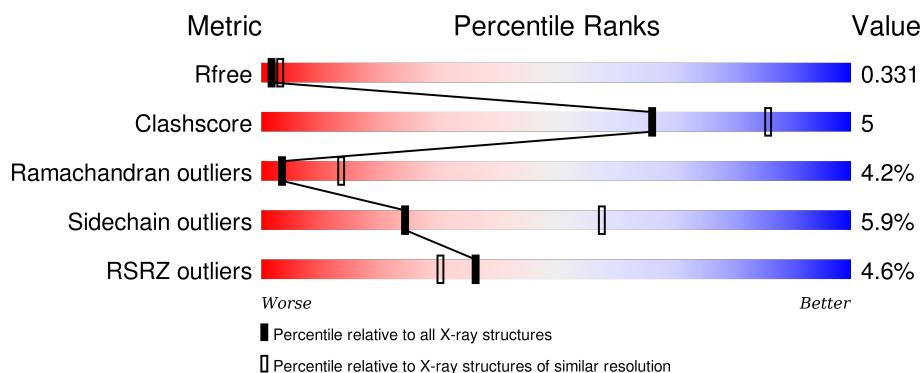
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	258	 3% 61% 14% • 23%
1	B	258	 2% 62% 14% • 23%
1	C	258	 3% 62% 16% • 21%
1	D	258	 6% 65% 10% • 24%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6256 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 Retinoid X receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1505	963	261	274	7			
1	B	198	Total	C	N	O	S	0	0	0
			1522	975	266	272	9			
1	C	203	Total	C	N	O	S	0	0	0
			1566	1001	276	281	8			
1	D	197	Total	C	N	O	S	0	0	0
			1488	941	265	274	8			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	80	MET	-	EXPRESSION TAG	UNP Q9UAF1
A	81	GLY	-	EXPRESSION TAG	UNP Q9UAF1
A	82	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	83	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	84	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	85	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	86	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	87	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	88	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	89	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	90	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	91	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	92	GLY	-	EXPRESSION TAG	UNP Q9UAF1
A	93	LEU	-	EXPRESSION TAG	UNP Q9UAF1
A	94	VAL	-	EXPRESSION TAG	UNP Q9UAF1
A	95	PRO	-	EXPRESSION TAG	UNP Q9UAF1
A	96	ARG	-	EXPRESSION TAG	UNP Q9UAF1
A	97	GLY	-	EXPRESSION TAG	UNP Q9UAF1
A	98	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	99	HIS	-	EXPRESSION TAG	UNP Q9UAF1
A	100	MET	-	EXPRESSION TAG	UNP Q9UAF1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	-	EXPRESSION TAG	UNP Q9UAF1
A	102	SER	-	EXPRESSION TAG	UNP Q9UAF1
A	248	VAL	ILE	ENGINEERED	UNP Q9UAF1
A	258	PRO	LEU	ENGINEERED	UNP Q9UAF1
B	80	MET	-	EXPRESSION TAG	UNP Q9UAF1
B	81	GLY	-	EXPRESSION TAG	UNP Q9UAF1
B	82	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	83	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	84	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	85	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	86	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	87	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	88	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	89	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	90	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	91	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	92	GLY	-	EXPRESSION TAG	UNP Q9UAF1
B	93	LEU	-	EXPRESSION TAG	UNP Q9UAF1
B	94	VAL	-	EXPRESSION TAG	UNP Q9UAF1
B	95	PRO	-	EXPRESSION TAG	UNP Q9UAF1
B	96	ARG	-	EXPRESSION TAG	UNP Q9UAF1
B	97	GLY	-	EXPRESSION TAG	UNP Q9UAF1
B	98	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	99	HIS	-	EXPRESSION TAG	UNP Q9UAF1
B	100	MET	-	EXPRESSION TAG	UNP Q9UAF1
B	101	ALA	-	EXPRESSION TAG	UNP Q9UAF1
B	102	SER	-	EXPRESSION TAG	UNP Q9UAF1
B	248	VAL	ILE	ENGINEERED	UNP Q9UAF1
B	258	PRO	LEU	ENGINEERED	UNP Q9UAF1
C	80	MET	-	EXPRESSION TAG	UNP Q9UAF1
C	81	GLY	-	EXPRESSION TAG	UNP Q9UAF1
C	82	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	83	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	84	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	85	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	86	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	87	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	88	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	89	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	90	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	91	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	92	GLY	-	EXPRESSION TAG	UNP Q9UAF1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	LEU	-	EXPRESSION TAG	UNP Q9UAF1
C	94	VAL	-	EXPRESSION TAG	UNP Q9UAF1
C	95	PRO	-	EXPRESSION TAG	UNP Q9UAF1
C	96	ARG	-	EXPRESSION TAG	UNP Q9UAF1
C	97	GLY	-	EXPRESSION TAG	UNP Q9UAF1
C	98	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	99	HIS	-	EXPRESSION TAG	UNP Q9UAF1
C	100	MET	-	EXPRESSION TAG	UNP Q9UAF1
C	101	ALA	-	EXPRESSION TAG	UNP Q9UAF1
C	102	SER	-	EXPRESSION TAG	UNP Q9UAF1
C	248	VAL	ILE	ENGINEERED	UNP Q9UAF1
C	258	PRO	LEU	ENGINEERED	UNP Q9UAF1
D	80	MET	-	EXPRESSION TAG	UNP Q9UAF1
D	81	GLY	-	EXPRESSION TAG	UNP Q9UAF1
D	82	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	83	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	84	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	85	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	86	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	87	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	88	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	89	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	90	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	91	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	92	GLY	-	EXPRESSION TAG	UNP Q9UAF1
D	93	LEU	-	EXPRESSION TAG	UNP Q9UAF1
D	94	VAL	-	EXPRESSION TAG	UNP Q9UAF1
D	95	PRO	-	EXPRESSION TAG	UNP Q9UAF1
D	96	ARG	-	EXPRESSION TAG	UNP Q9UAF1
D	97	GLY	-	EXPRESSION TAG	UNP Q9UAF1
D	98	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	99	HIS	-	EXPRESSION TAG	UNP Q9UAF1
D	100	MET	-	EXPRESSION TAG	UNP Q9UAF1
D	101	ALA	-	EXPRESSION TAG	UNP Q9UAF1
D	102	SER	-	EXPRESSION TAG	UNP Q9UAF1
D	248	VAL	ILE	ENGINEERED	UNP Q9UAF1
D	258	PRO	LEU	ENGINEERED	UNP Q9UAF1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	49	Total O 49 49	0	0

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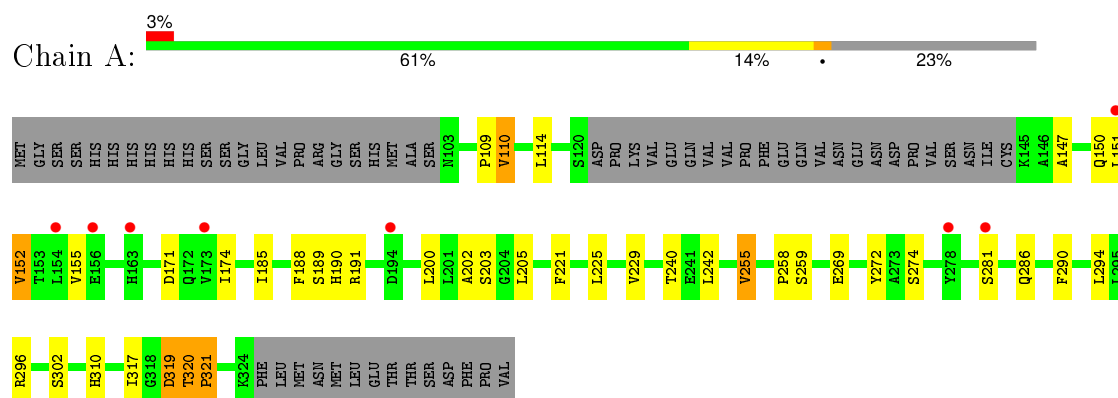
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	42	Total 42	O 42	0	0
2	C	47	Total 47	O 47	0	0
2	D	37	Total 37	O 37	0	0

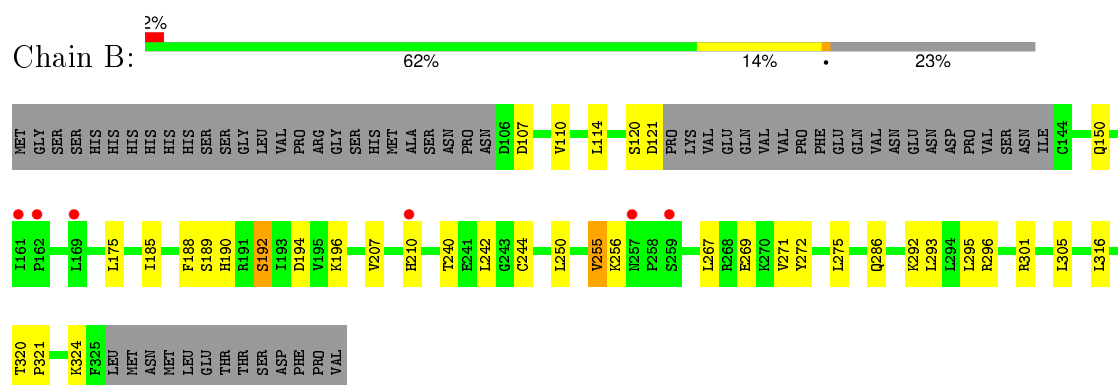
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

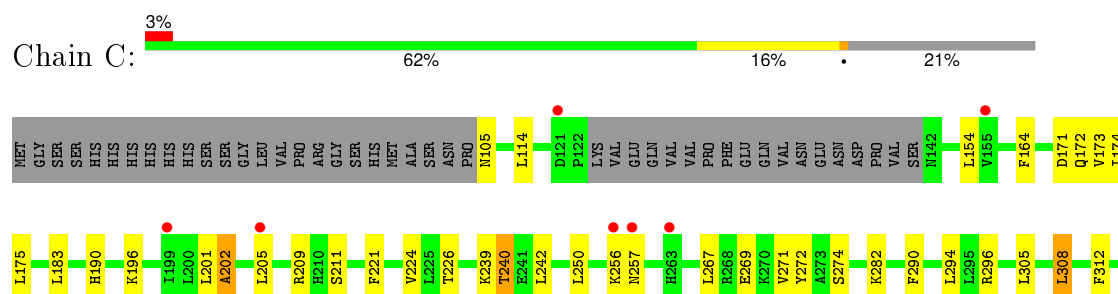
#### • Molecule 1: Retinoid X receptor

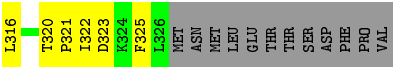


#### • Molecule 1: Retinoid X receptor

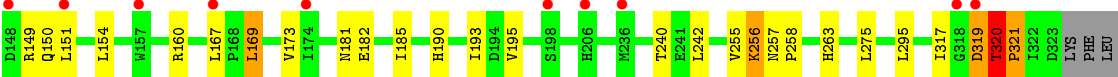


#### • Molecule 1: Retinoid X receptor





● Molecule 1: Retinoid X receptor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.26 Å 96.12 Å 151.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.90 48.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.22-2.90) 99.5 (48.24-2.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.34 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.269 , 0.325 0.268 , 0.331	Depositor DCC
$R_{free}$ test set	1361 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 76.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 27210 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7349e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.32	0/1537	0.50	0/2085
1	B	0.30	0/1554	0.47	0/2103
1	C	0.31	0/1599	0.53	0/2163
1	D	0.31	0/1519	0.50	0/2057
All	All	0.31	0/6209	0.50	0/8408

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	THR	Peptide
1	D	320	THR	Peptide

### 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	1505	0	1471	19	0
1	B	1522	0	1497	14	0
1	C	1566	0	1539	18	0
1	D	1488	0	1431	11	0
2	A	49	0	0	1	0
2	B	42	0	0	0	0
2	C	47	0	0	0	0
2	D	37	0	0	0	0
All	All	6256	0	5938	59	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 5.

All (59) 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:190:HIS:CG	1:D:242:LEU:HD22	2.38	0.58
1:C:164:PHE:HE1	1:C:175:LEU:HD11	1.70	0.55
1:A:109:PRO:O	1:A:110:VAL:HB	2.07	0.55
1:C:269:GLU:HA	1:C:272:TYR:CE1	2.41	0.55
1:A:190:HIS:CD2	1:A:242:LEU:HD22	2.42	0.55
1:C:114:LEU:HG	1:C:240:THR:HG22	1.91	0.51
1:B:267:LEU:O	1:B:271:VAL:HG23	2.10	0.51
1:A:310:HIS:CD2	1:C:308:LEU:HD22	2.45	0.51
1:C:322:ILE:HG23	1:C:322:ILE:O	2.10	0.51
1:A:302:SER:HB2	1:B:301:ARG:HD3	1.92	0.51
1:D:167:LEU:HD23	1:D:263:HIS:CE1	2.46	0.50
1:A:152:VAL:HG12	1:A:155:VAL:HG23	1.93	0.50
1:D:319:ASP:O	1:D:320:THR:HG23	2.12	0.49
1:B:292:LYS:O	1:B:293:LEU:HB2	2.12	0.49
1:D:182:GLU:HA	1:D:185:ILE:HG22	1.93	0.49
1:C:290:PHE:CZ	1:C:294:LEU:HD11	2.47	0.49
1:C:209:ARG:HA	1:C:221:PHE:CE2	2.47	0.49
1:C:105:ASN:N	1:C:274:SER:HG	2.10	0.49
1:A:320:THR:HA	1:A:321:PRO:C	2.33	0.48
1:A:221:PHE:CE2	1:A:225:LEU:HD11	2.48	0.48
1:B:207:VAL:HG21	1:B:316:LEU:HB2	1.95	0.48
1:B:185:ILE:HA	1:B:188:PHE:CE2	2.48	0.48
1:A:225:LEU:HA	1:A:229:VAL:HG22	1.96	0.47
1:C:190:HIS:CG	1:C:242:LEU:HD22	2.50	0.47
1:C:256:LYS:C	1:C:257:ASN:HD22	2.19	0.46
1:D:320:THR:HA	1:D:321:PRO:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CZ	1:A:294:LEU:HD11	2.51	0.46
1:A:269:GLU:HA	1:A:272:TYR:CZ	2.50	0.46
1:C:175:LEU:HD13	1:C:250:LEU:O	2.16	0.45
1:A:319:ASP:O	1:A:320:THR:C	2.54	0.45
1:B:175:LEU:HD23	1:B:255:VAL:HG21	1.99	0.45
1:B:269:GLU:HA	1:B:272:TYR:CE1	2.52	0.44
1:B:190:HIS:CD2	1:B:242:LEU:HD22	2.52	0.44
1:C:154:LEU:HD21	1:C:183:LEU:HD13	1.99	0.43
1:B:292:LYS:O	1:B:293:LEU:CB	2.67	0.43
1:A:191:ARG:NH2	1:A:202:ALA:HB2	2.34	0.43
1:C:320:THR:HA	1:C:322:ILE:N	2.34	0.42
1:B:192:SER:O	1:B:194:ASP:N	2.50	0.42
1:A:286:GLN:NE2	2:A:377:HOH:O	2.51	0.42
1:A:185:ILE:HA	1:A:188:PHE:CE2	2.54	0.42
1:D:119:ILE:HD11	1:D:160:ARG:HG3	2.02	0.41
1:B:175:LEU:HD22	1:B:250:LEU:O	2.19	0.41
1:A:296:ARG:NE	1:A:296:ARG:HA	2.35	0.41
1:B:292:LYS:HD3	1:B:295:LEU:HB2	2.03	0.41
1:C:171:ASP:HA	1:C:174:ILE:HG12	2.03	0.41
1:D:257:ASN:N	1:D:258:PRO:HD3	2.36	0.41
1:A:174:ILE:HG22	1:A:255:VAL:HG21	2.02	0.41
1:B:275:LEU:HD11	1:B:293:LEU:HD13	2.02	0.41
1:D:255:VAL:HG13	1:D:255:VAL:O	2.21	0.41
1:D:256:LYS:HE2	1:D:256:LYS:HA	2.02	0.41
1:C:267:LEU:O	1:C:271:VAL:HG23	2.21	0.40
1:A:110:VAL:HG23	1:A:274:SER:HB3	2.02	0.40
1:C:294:LEU:HD22	1:D:295:LEU:HD21	2.03	0.40
1:C:312:PHE:CE2	1:C:316:LEU:HD11	2.56	0.40
1:C:201:LEU:O	1:C:202:ALA:C	2.59	0.40
1:A:109:PRO:O	1:A:110:VAL:CB	2.68	0.40
1:A:189:SER:HA	1:A:229:VAL:HG12	2.04	0.40
1:D:169:LEU:O	1:D:173:VAL:HG23	2.21	0.40
1:B:110:VAL:HG23	1:B:244:CYS:SG	2.61	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	194/258 (75%)	161 (83%)	21 (11%)	12 (6%)	2	5
1	B	194/258 (75%)	173 (89%)	14 (7%)	7 (4%)	4	18
1	C	199/258 (77%)	175 (88%)	16 (8%)	8 (4%)	4	15
1	D	193/258 (75%)	173 (90%)	14 (7%)	6 (3%)	5	21
All	All	780/1032 (76%)	682 (87%)	65 (8%)	33 (4%)	3	13

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ALA
1	A	203	SER
1	A	319	ASP
1	A	321	PRO
1	B	120	SER
1	B	192	SER
1	C	173	VAL
1	C	202	ALA
1	C	321	PRO
1	D	317	ILE
1	D	321	PRO
1	A	205	LEU
1	A	259	SER
1	A	281	SER
1	C	211	SER
1	C	224	VAL
1	D	150	GLN
1	B	150	GLN
1	B	196	LYS
1	C	172	GLN
1	D	147	ALA
1	A	110	VAL

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Mol	Chain	Res	Type
1	A	200	LEU
1	A	258	PRO
1	B	256	LYS
1	B	321	PRO
1	C	205	LEU
1	C	282	LYS
1	D	319	ASP
1	A	317	ILE
1	A	152	VAL
1	B	255	VAL
1	D	104	PRO

### 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	158/231 (68%)	152 (96%)	6 (4%)	40	76
1	B	157/231 (68%)	146 (93%)	11 (7%)	19	47
1	C	163/231 (71%)	154 (94%)	9 (6%)	27	61
1	D	154/231 (67%)	143 (93%)	11 (7%)	18	47
All	All	632/924 (68%)	595 (94%)	37 (6%)	24	58

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	150	GLN
1	A	151	LEU
1	A	171	ASP
1	A	240	THR
1	A	255	VAL
1	B	107	ASP
1	B	114	LEU
1	B	121	ASP
1	B	189	SER

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Mol	Chain	Res	Type
1	B	210	HIS
1	B	240	THR
1	B	286	GLN
1	B	296	ARG
1	B	305	LEU
1	B	320	THR
1	B	324	LYS
1	C	196	LYS
1	C	226	THR
1	C	239	LYS
1	C	240	THR
1	C	296	ARG
1	C	305	LEU
1	C	308	LEU
1	C	323	ASP
1	C	325	PHE
1	D	149	ARG
1	D	151	LEU
1	D	154	LEU
1	D	169	LEU
1	D	181	ASN
1	D	193	ILE
1	D	195	VAL
1	D	240	THR
1	D	256	LYS
1	D	275	LEU
1	D	320	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	286	GLN
1	B	181	ASN
1	B	190	HIS
1	B	214	GLN
1	C	142	ASN
1	C	172	GLN
1	C	257	ASN
1	C	286	GLN
1	D	103	ASN
1	D	172	GLN

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Mol	Chain	Res	Type
1	D	181	ASN

### 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](#)

There are no ligands in this entry.

### 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, 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	198/258 (76%)	0.37	8 (4%)	42	35	41, 60, 80, 85	1 (0%)
1	B	198/258 (76%)	0.30	6 (3%)	54	47	43, 66, 78, 81	0
1	C	203/258 (78%)	0.39	7 (3%)	49	41	41, 62, 73, 77	0
1	D	197/258 (76%)	0.46	16 (8%)	15	9	46, 67, 85, 94	0
All	All	796/1032 (77%)	0.38	37 (4%)	36	30	41, 64, 82, 94	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	151	LEU	3.4
1	C	155	VAL	3.1
1	D	148	ASP	3.0
1	A	154	LEU	2.9
1	A	163	HIS	2.9
1	D	318	GLY	2.8
1	B	161	ILE	2.8
1	D	113	ILE	2.7
1	B	259	SER	2.6
1	D	157	TRP	2.6
1	D	104	PRO	2.4
1	D	198	SER	2.3
1	B	169	LEU	2.3
1	D	206	HIS	2.3
1	C	257	ASN	2.3
1	A	173	VAL	2.3
1	A	281	SER	2.2
1	D	110	VAL	2.2
1	C	205	LEU	2.2
1	D	236	MET	2.2
1	B	162	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	210	HIS	2.1
1	D	116	ALA	2.1
1	C	199	ILE	2.1
1	D	119	ILE	2.1
1	D	174	ILE	2.1
1	C	256	LYS	2.1
1	D	167	LEU	2.1
1	C	121	ASP	2.1
1	A	151	LEU	2.1
1	C	263	HIS	2.1
1	D	319	ASP	2.1
1	B	257	ASN	2.1
1	A	156	GLU	2.0
1	A	194	ASP	2.0
1	A	278	TYR	2.0
1	D	103	ASN	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.