



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:27 PM UTC

PDB ID : 2Q60 / pdb_00002q60
Title : Crystal structure of the ligand binding domain of polyandrocampa 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

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:

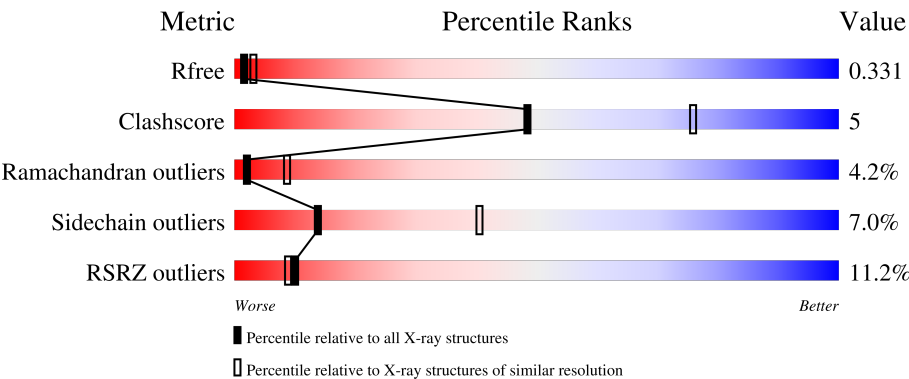
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	258	9% 59%15%•23%
1	B	258	6% 62%14%•23%
1	C	258	5% 62%14%•21%
1	D	258	14% 64%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 mutation	UNP Q9UAF1
A	258	PRO	LEU	engineered mutation	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 mutation	UNP Q9UAF1
B	258	PRO	LEU	engineered mutation	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 mutation	UNP Q9UAF1
C	258	PRO	LEU	engineered mutation	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 mutation	UNP Q9UAF1
D	258	PRO	LEU	engineered mutation	UNP Q9UAF1

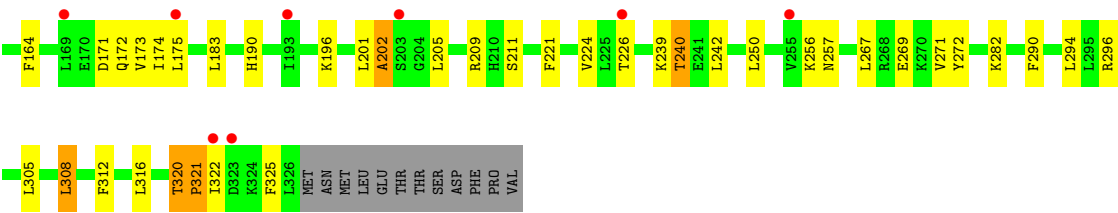
- Molecule 2 is water.

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

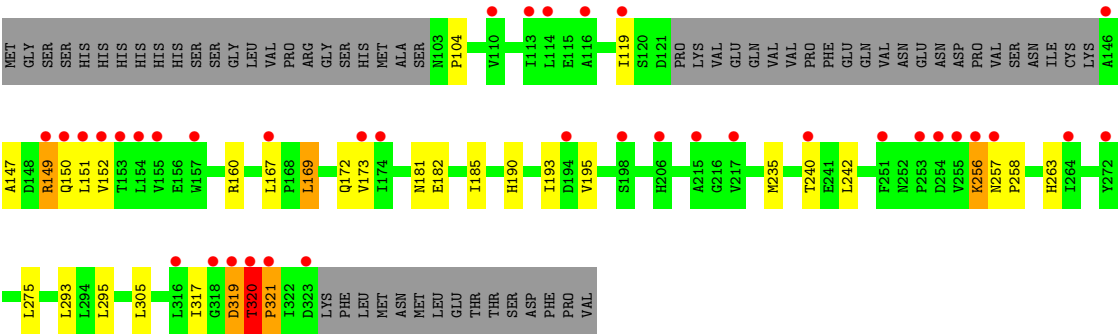
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	42	Total 42	O 42	0	0
2	C	47	Total 47	O 47	0	0
2	D	37	Total 37	O 37	0	0



● 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, α , β , γ	82.26Å 96.12Å 151.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.90 48.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.22-2.90) 99.4 (48.22-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.91Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.269 , 0.325 0.269 , 0.331	Depositor DCC
R_{free} test set	1361 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6256	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage'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.*

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

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	0.47	0/1537	0.78	2/2085 (0.1%)
1	B	0.44	0/1554	0.74	0/2103
1	C	0.45	0/1599	0.77	2/2163 (0.1%)
1	D	0.46	0/1519	0.77	1/2057 (0.0%)
All	All	0.46	0/6209	0.76	5/8408 (0.1%)

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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	108	MET	CA-C-N	5.33	126.50	119.84
1	A	108	MET	C-N-CA	5.33	126.50	119.84
1	C	320	THR	CA-C-N	5.22	139.52	127.00
1	C	320	THR	C-N-CA	5.22	139.52	127.00
1	D	149	ARG	N-CA-C	5.04	115.95	108.60

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 ⓘ

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	22	0
1	B	1522	0	1497	16	0
1	C	1566	0	1539	19	0
1	D	1488	0	1431	12	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	66	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 (66) 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:A:235:MET:HE1	1:A:293:LEU:CD2	2.35	0.56
1:D:235:MET:HE1	1:D:293:LEU:HD11	1.86	0.56
1:D:235:MET:HE1	1:D:293:LEU:CD1	2.35	0.56
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:A:320:THR:HA	1:A:321:PRO:C	2.33	0.53
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:C:256:LYS:C	1:C:257:ASN:HD22	2.19	0.51
1:A:302:SER:HB2	1:B:301:ARG:HD3	1.92	0.51
1:D:320:THR:HA	1:D:321:PRO:C	2.36	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:A:319:ASP:O	1:A:320:THR:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LYS:O	1:B:293:LEU:HB2	2.12	0.49
1:D:319:ASP:O	1:D:320:THR:HG23	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:A:235:MET:HE1	1:A:293:LEU:HD23	1.95	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: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:C:201:LEU:O	1:C:202:ALA:C	2.59	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:C:320:THR:HA	1:C:321:PRO:C	2.42	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:235:MET:HE1	1:A:293:LEU:HD21	1.99	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:B:235:MET:HE1	1:B:293:LEU:CD2	2.49	0.42
1:C:175:LEU:C	1:C:175:LEU:HD12	2.45	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:A:174:ILE:HG22	1:A:255:VAL:HG21	2.02	0.41
1:D:257:ASN:N	1:D:258:PRO:HD3	2.36	0.41
1:B:275:LEU:HD11	1:B:293:LEU:HD13	2.02	0.41
1:D:256:LYS:HA	1:D:256:LYS:HE2	2.02	0.41
1:B:237:MET:HE2	1:B:293:LEU:HD23	2.04	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:110:VAL:HG23	1:B:244:CYS:SG	2.61	0.40
1:D:169:LEU:O	1:D:173:VAL:HG23	2.21	0.40

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	194/258 (75%)	161 (83%)	21 (11%)	12 (6%)	1	3
1	B	194/258 (75%)	173 (89%)	14 (7%)	7 (4%)	2	11
1	C	199/258 (77%)	175 (88%)	16 (8%)	8 (4%)	2	9
1	D	193/258 (75%)	173 (90%)	14 (7%)	6 (3%)	3	14
All	All	780/1032 (76%)	682 (87%)	65 (8%)	33 (4%)	2	9

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

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Mol	Chain	Res	Type
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
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%)	149 (94%)	9 (6%)	18	49
1	B	157/231 (68%)	145 (92%)	12 (8%)	12	36
1	C	163/231 (71%)	153 (94%)	10 (6%)	17	46
1	D	154/231 (67%)	141 (92%)	13 (8%)	10	31
All	All	632/924 (68%)	588 (93%)	44 (7%)	14	40

All (44) 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	208	HIS
1	A	229	VAL
1	A	240	THR
1	A	255	VAL
1	A	275	LEU
1	A	305	LEU
1	B	114	LEU
1	B	189	SER
1	B	200	LEU
1	B	201	LEU
1	B	210	HIS
1	B	240	THR
1	B	255	VAL
1	B	275	LEU
1	B	286	GLN
1	B	296	ARG
1	B	305	LEU
1	B	320	THR
1	C	114	LEU
1	C	118	LEU
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	325	PHE
1	D	149	ARG
1	D	151	LEU
1	D	152	VAL
1	D	169	LEU
1	D	172	GLN
1	D	181	ASN
1	D	193	ILE
1	D	195	VAL
1	D	240	THR
1	D	256	LYS
1	D	275	LEU

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Mol	Chain	Res	Type
1	D	305	LEU
1	D	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	286	GLN
1	B	190	HIS
1	B	208	HIS
1	B	214	GLN
1	B	286	GLN
1	C	142	ASN
1	C	208	HIS
1	C	257	ASN
1	C	286	GLN
1	D	103	ASN
1	D	172	GLN
1	D	181	ASN
1	D	210	HIS
1	D	286	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 oligosaccharides 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, 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	198/258 (76%)	0.85	24 (12%) 8 7	31, 59, 80, 85	1 (0%)
1	B	198/258 (76%)	0.94	15 (7%) 20 16	43, 66, 78, 81	0
1	C	203/258 (78%)	0.82	13 (6%) 25 20	41, 62, 73, 77	0
1	D	197/258 (76%)	1.22	37 (18%) 3 3	46, 67, 85, 94	0
All	All	796/1032 (77%)	0.96	89 (11%) 10 9	31, 64, 82, 94	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	HIS	7.8
1	D	318	GLY	4.6
1	D	152	VAL	4.0
1	D	198	SER	3.7
1	A	152	VAL	3.7
1	D	110	VAL	3.6
1	D	256	LYS	3.5
1	D	194	ASP	3.4
1	A	280	ARG	3.4
1	B	322	ILE	3.4
1	D	320	THR	3.4
1	D	155	VAL	3.4
1	D	206	HIS	3.3
1	A	163	HIS	3.3
1	D	116	ALA	3.3
1	C	110	VAL	3.2
1	C	203	SER	3.2
1	D	119	ILE	3.2
1	D	114	LEU	3.1
1	D	151	LEU	3.0
1	C	255	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	217	VAL	3.0
1	B	210	HIS	2.9
1	C	322	ILE	2.9
1	D	146	ALA	2.8
1	D	255	VAL	2.8
1	C	143	ILE	2.8
1	C	175	LEU	2.8
1	A	320	THR	2.8
1	D	321	PRO	2.8
1	D	150	GLN	2.7
1	A	154	LEU	2.7
1	B	226	THR	2.7
1	D	319	ASP	2.7
1	D	157	TRP	2.7
1	D	254	ASP	2.7
1	B	151	LEU	2.6
1	C	152	VAL	2.6
1	D	316	LEU	2.5
1	B	285	ASP	2.5
1	B	198	SER	2.5
1	D	253	PRO	2.5
1	A	150	GLN	2.5
1	B	281	SER	2.4
1	A	258	PRO	2.4
1	C	323	ASP	2.4
1	D	264	ILE	2.4
1	D	323	ASP	2.4
1	A	110	VAL	2.4
1	D	272	TYR	2.4
1	B	162	PRO	2.4
1	A	321	PRO	2.4
1	B	144	CYS	2.3
1	A	206	HIS	2.3
1	B	293	LEU	2.3
1	A	104	PRO	2.3
1	D	167	LEU	2.3
1	A	157	TRP	2.3
1	D	257	ASN	2.3
1	A	194	ASP	2.3
1	D	154	LEU	2.3
1	D	240	THR	2.3
1	C	142	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	226	THR	2.2
1	A	119	ILE	2.2
1	A	145	LYS	2.2
1	B	201	LEU	2.2
1	C	169	LEU	2.2
1	B	260	ASP	2.2
1	D	153	THR	2.2
1	D	149	ARG	2.2
1	D	174	ILE	2.2
1	A	318	GLY	2.2
1	A	120	SER	2.2
1	A	221	PHE	2.2
1	A	146	ALA	2.2
1	A	291	ALA	2.2
1	C	193	ILE	2.1
1	A	151	LEU	2.1
1	D	113	ILE	2.1
1	D	173	VAL	2.1
1	B	121	ASP	2.1
1	B	220	ILE	2.1
1	D	251	PHE	2.0
1	C	146	ALA	2.0
1	A	166	SER	2.0
1	A	198	SER	2.0
1	B	316	LEU	2.0
1	D	215	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.