



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:47 am BST

PDB ID : 2GL8  
Title : Human Retinoic acid receptor RXR-gamma ligand-binding domain  
Authors : Min, J.R.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-04-04  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

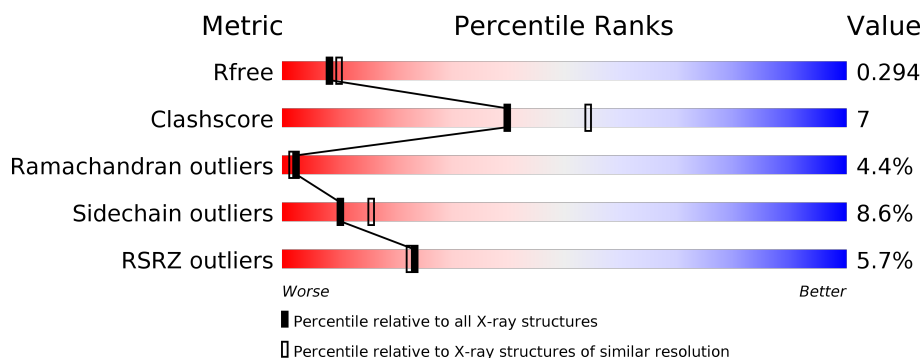
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	241	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>20%</div> <div>5%</div> <div>21%</div> </div> </div>
1	B	241	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>17%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	241	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>14%</div> <div>••</div> <div>20%</div> </div> </div>
1	D	241	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>••</div> <div>19%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5916 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 Retinoic acid receptor RXR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1459	931	254	268	6			
1	B	192	Total	C	N	O	S	0	0	0
			1454	928	257	263	6			
1	C	194	Total	C	N	O	S	0	0	0
			1447	919	256	266	6			
1	D	195	Total	C	N	O	S	0	0	0
			1451	920	254	271	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P48443
A	2	SER	-	CLONING ARTIFACT	UNP P48443
A	3	HIS	-	CLONING ARTIFACT	UNP P48443
A	4	ASN	-	CLONING ARTIFACT	UNP P48443
B	1	GLY	-	CLONING ARTIFACT	UNP P48443
B	2	SER	-	CLONING ARTIFACT	UNP P48443
B	3	HIS	-	CLONING ARTIFACT	UNP P48443
B	4	ASN	-	CLONING ARTIFACT	UNP P48443
C	1	GLY	-	CLONING ARTIFACT	UNP P48443
C	2	SER	-	CLONING ARTIFACT	UNP P48443
C	3	HIS	-	CLONING ARTIFACT	UNP P48443
C	4	ASN	-	CLONING ARTIFACT	UNP P48443
D	1	GLY	-	CLONING ARTIFACT	UNP P48443
D	2	SER	-	CLONING ARTIFACT	UNP P48443
D	3	HIS	-	CLONING ARTIFACT	UNP P48443
D	4	ASN	-	CLONING ARTIFACT	UNP P48443

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	B	23	Total 23	O 23	0	0
2	C	27	Total 27	O 27	0	0
2	D	23	Total 23	O 23	0	0

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

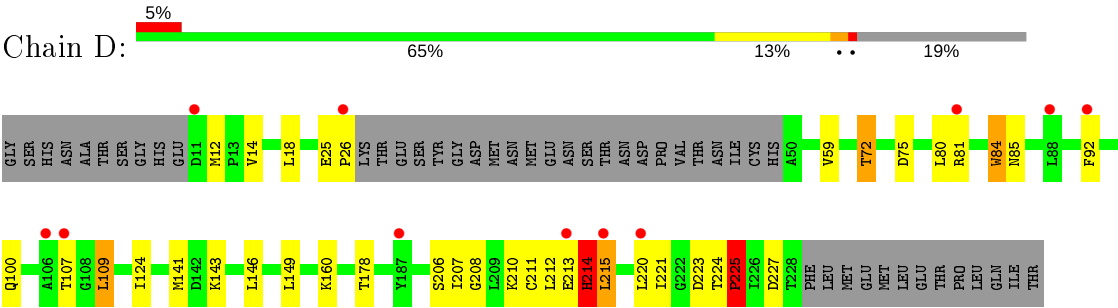
- Chain A:
- 
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.25). The x-axis shows positions 1 to 222. A color scale at the top indicates conservation levels: 6% (red), 55% (green), 20% (yellow), 5% (orange), and 21% (grey).
- Key residues and conservation levels (approximate):
- Position 1: GLY (0.25 bits)
  - Position 2: SER (0.25 bits)
  - Position 3: HIS (0.25 bits)
  - Position 4: ASN (0.25 bits)
  - Position 5: ALA (0.25 bits)
  - Position 6: THR (0.25 bits)
  - Position 7: SER (0.25 bits)
  - Position 8: GLY (0.25 bits)
  - Position 9: HIS (0.25 bits)
  - Position 10: GLU (0.25 bits)
  - Position 11: D11 (0.25 bits)
  - Position 12: Y14 (0.25 bits)
  - Position 13: L18 (0.25 bits)
  - Position 14: E21 (0.25 bits)
  - Position 15: L22 (0.25 bits)
  - Position 16: E25 (0.25 bits)
  - Position 17: PRO (0.25 bits)
  - Position 18: LYS (0.25 bits)
  - Position 19: THR (0.25 bits)
  - Position 20: THR (0.25 bits)
  - Position 21: GLU (0.25 bits)
  - Position 22: SER (0.25 bits)
  - Position 23: MET (0.25 bits)
  - Position 24: ASP (0.25 bits)
  - Position 25: GLY (0.25 bits)
  - Position 26: TYR (0.25 bits)
  - Position 27: TLR (0.25 bits)
  - Position 28: ASN (0.25 bits)
  - Position 29: ASN (0.25 bits)
  - Position 30: MET (0.25 bits)
  - Position 31: ASP (0.25 bits)
  - Position 32: ASP (0.25 bits)
  - Position 33: PRO (0.25 bits)
  - Position 34: VAL (0.25 bits)
  - Position 35: THR (0.25 bits)
  - Position 36: THR (0.25 bits)
  - Position 37: ASN (0.25 bits)
  - Position 38: ILE (0.25 bits)
  - Position 39: CYS (0.25 bits)
  - Position 40: HIS (0.25 bits)
  - Position 41: A50 (0.25 bits)
  - Position 42: A51 (0.25 bits)
  - Position 43: D52 (0.25 bits)
  - Position 44: K53 (0.25 bits)
  - Position 45: Q54 (0.25 bits)
  - Position 46: L55 (0.25 bits)
  - Position 47: F56 (0.25 bits)
  - Position 48: T57 (0.25 bits)
  - Position 49: L58 (0.25 bits)
  - Position 50: V59 (0.25 bits)
  - Position 51: K63 (0.25 bits)
  - Position 52: S69 (0.25 bits)
  - Position 53: T72 (0.25 bits)
  - Position 54: L73 (0.25 bits)
  - Position 55: E74 (0.25 bits)
  - Position 56: D75 (0.25 bits)
  - Position 57: L80 (0.25 bits)
  - Position 58: R81 (0.25 bits)
  - Position 59: L87 (0.25 bits)
  - Position 60: L88 (0.25 bits)
  - Position 61: F92 (0.25 bits)
  - Position 62: S93 (0.25 bits)
  - Position 63: R94 (0.25 bits)
  - Position 64: R95 (0.25 bits)
  - Position 65: Q100 (0.25 bits)
  - Position 66: D101 (0.25 bits)
  - Position 67: G102 (0.25 bits)
  - Position 68: I103 (0.25 bits)
  - Position 69: L104 (0.25 bits)
  - Position 70: L105 (0.25 bits)
  - Position 71: A106 (0.25 bits)
  - Position 72: T107 (0.25 bits)
  - Position 73: G108 (0.25 bits)
  - Position 74: L109 (0.25 bits)
  - Position 75: H110 (0.25 bits)
  - Position 76: V111 (0.25 bits)
  - Position 77: H112 (0.25 bits)
  - Position 78: R113 (0.25 bits)
  - Position 79: T124 (0.25 bits)
  - Position 80: F125 (0.25 bits)
  - Position 81: D126 (0.25 bits)
  - Position 82: M141 (0.25 bits)
  - Position 83: L146 (0.25 bits)
  - Position 84: G147 (0.25 bits)
  - Position 85: K160 (0.25 bits)
  - Position 86: N164 (0.25 bits)
  - Position 87: E167 (0.25 bits)
  - Position 88: E173 (0.25 bits)
  - Position 89: Y176 (0.25 bits)
  - Position 90: A177 (0.25 bits)
  - Position 91: T178 (0.25 bits)
  - Position 92: L179 (0.25 bits)
  - Position 93: E180 (0.25 bits)
  - Position 94: A181 (0.25 bits)
  - Position 95: Y182 (0.25 bits)
  - Position 96: K184 (0.25 bits)
  - Position 97: Q185 (0.25 bits)
  - Position 98: F194 (0.25 bits)

- Chain B:
- 
- | Residue | Conservation |
|---------|--------------|
| GLY     | Conserved    |
| SER     | Conserved    |
| HIS     | Conserved    |
| ASN     | Conserved    |
| ALA     | Conserved    |
| THR     | Conserved    |
| SER     | Conserved    |
| GLY     | Conserved    |
| HIS     | Conserved    |
| GLU     | Conserved    |
| D11     | Conserved    |
| V14     | Conserved    |
| E15     | Conserved    |
| R16     | Conserved    |
| I17     | Conserved    |
| L18     | Conserved    |
| E25     | Conserved    |
| PRO     | Conserved    |
| LYS     | Conserved    |
| THR     | Conserved    |
| GLU     | Conserved    |
| SER     | Conserved    |
| TYR     | Conserved    |
| GLY     | Conserved    |
| ASP     | Conserved    |
| MET     | Conserved    |
| ASN     | Conserved    |
| MET     | Conserved    |
| GLU     | Conserved    |
| ASN     | Conserved    |
| SER     | Conserved    |
| THR     | Conserved    |
| THR     | Conserved    |
| ASP     | Conserved    |
| PRO     | Conserved    |
| VAL     | Conserved    |
| THR     | Conserved    |
| ILE     | Conserved    |
| CYS     | Conserved    |
| HIS     | Conserved    |
| A50     | Conserved    |
| A51     | Conserved    |
| D52     | Conserved    |
| K63     | Conserved    |
| Q64     | Conserved    |
| L55     | Conserved    |
| F56     | Conserved    |
| T57     | Conserved    |
| W61     | Conserved    |
| P66     | Conserved    |
| D70     | Conserved    |
| L73     | Conserved    |
| V99     | Conserved    |
| L104    | Conserved    |
| L106    | Conserved    |
| L107    | Conserved    |
| R113    | Conserved    |
| S114    | Conserved    |
| H117    | Conserved    |
| L129    | Conserved    |
| V133    | Conserved    |
| M141    | Conserved    |
| L146    | Conserved    |
| L154    | Conserved    |
| K160    | Conserved    |
| M164    | Conserved    |
| E167    | Conserved    |
| V168    | Conserved    |
| E169    | Conserved    |
| V175    | Conserved    |
| V176    | Conserved    |
| L179    | Conserved    |
| E180    | Conserved    |
| T183    | Conserved    |
| F194    | Conserved    |
| A195    | Conserved    |
| K196    | Conserved    |
| L197    | Conserved    |
| L209    | Conserved    |
| K210    | Conserved    |
| G211    | Conserved    |
| L212    | Conserved    |
| E213    | Conserved    |
| E214    | Conserved    |
| L215    | Conserved    |
| F216    | Conserved    |
| F217    | Conserved    |
| L220    | Conserved    |
| L221    | Conserved    |
| G222    | Conserved    |
| D223    | Conserved    |
| T224    | Conserved    |
| P225    | Conserved    |
| T226    | Conserved    |

- Chain C:
- 
- | Amino Acid | Percentage |
|------------|------------|
| GLY        | 20%        |
| SER        | 20%        |
| HIS        | 20%        |
| ASN        | 20%        |
| ALA        | 20%        |
| THR        | 20%        |
| SER        | 20%        |
| GLY        | 20%        |
| HIS        | 20%        |
| GLU        | 20%        |
| D11        | 4%         |
| V14        | 14%        |
| L18        | 14%        |
| E25        | 63%        |
| P26        | 63%        |
| LYS        | 63%        |
| THR        | 63%        |
| GLU        | 63%        |
| SER        | 63%        |
| TYR        | 63%        |
| GLY        | 63%        |
| ASP        | 63%        |
| MET        | 63%        |
| ASN        | 63%        |
| MET        | 63%        |
| GLU        | 63%        |
| ASN        | 63%        |
| SER        | 63%        |
| THR        | 63%        |
| ASN        | 63%        |
| ASP        | 63%        |
| PRO        | 63%        |
| VAL        | 63%        |
| THR        | 63%        |
| ASN        | 63%        |
| ILE        | 63%        |
| CYS        | 63%        |
| HIS        | 63%        |
| A50        | 14%        |
| A51        | 14%        |
| D52        | 14%        |
| K53        | 14%        |
| Q54        | 14%        |
| L55        | 14%        |
| F56        | 14%        |
| T57        | 14%        |
| L58        | 14%        |
| V59        | 14%        |
| D75        | 4%         |
| W84        | 20%        |
| N85        | 20%        |
| L88        | 20%        |
| D101       | 20%        |

ILE  
THR

● Molecule 1: Retinoic acid receptor RXR-gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.07Å 161.32Å 68.68Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	80.58 – 2.40 44.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (80.58-2.40) 99.0 (44.81-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.243 , 0.296 0.242 , 0.294	Depositor DCC
$R_{free}$ test set	1936 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 82.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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, 0.333 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	0.69	2/1484 (0.1%)	0.77	2/2005 (0.1%)
1	B	0.77	3/1480 (0.2%)	0.67	0/2001
1	C	0.59	1/1473 (0.1%)	0.70	1/1989 (0.1%)
1	D	0.49	0/1475	0.67	2/1996 (0.1%)
All	All	0.64	6/5912 (0.1%)	0.70	5/7991 (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	B	0	2
1	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	ILE	C-O	18.41	1.58	1.23
1	A	224	THR	C-O	9.48	1.41	1.23
1	C	26	PRO	C-O	9.32	1.41	1.23
1	A	224	THR	CB-CG2	5.45	1.70	1.52
1	B	212	LEU	C-O	5.42	1.33	1.23
1	B	212	LEU	CG-CD2	5.22	1.71	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	225	PRO	N-CA-CB	8.21	113.15	103.30
1	C	215	LEU	CA-CB-CG	7.76	133.16	115.30
1	D	215	LEU	CA-CB-CG	6.14	129.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	224	THR	CA-CB-CG2	-5.31	104.97	112.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	HIS	Peptide
1	B	53	LYS	Peptide
1	B	54	GLN	Peptide
1	D	223	ASP	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	1459	0	1470	36	0
1	B	1454	0	1454	17	0
1	C	1447	0	1434	17	0
1	D	1451	0	1424	17	0
2	A	32	0	0	0	0
2	B	23	0	0	0	0
2	C	27	0	0	0	0
2	D	23	0	0	0	0
All	All	5916	0	5782	84	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 7.

All (84) 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:B:215:LEU:HG	1:B:216:PHE:H	1.35	0.89
1:A:219:LYS:HA	1:A:220:LEU:HB2	1.57	0.84
1:A:219:LYS:HA	1:A:220:LEU:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:HG22	1:A:75:ASP:H	1.51	0.76
1:A:219:LYS:CA	1:A:220:LEU:HB2	2.16	0.75
1:A:164:ASN:ND2	1:A:167:GLU:HG3	2.04	0.73
1:A:141:MET:HE1	1:A:146:LEU:HD13	1.73	0.70
1:B:215:LEU:HG	1:B:216:PHE:N	2.07	0.68
1:A:124:ILE:HD11	1:A:207:ILE:HG23	1.74	0.68
1:C:206:SER:O	1:C:210:LYS:HD2	1.93	0.68
1:B:183:THR:HG21	1:B:194:PHE:HB2	1.74	0.68
1:A:164:ASN:HD22	1:A:167:GLU:HG3	1.60	0.66
1:A:181:ALA:O	1:A:185:GLN:HG3	1.95	0.65
1:C:189:GLU:HG2	1:C:190:GLN:HG3	1.81	0.63
1:C:53:LYS:HA	1:C:55:LEU:H	1.62	0.63
1:A:103:ILE:HD12	1:A:125:PHE:CE2	2.35	0.61
1:A:14:VAL:HG22	1:A:178:THR:HG23	1.80	0.61
1:D:141:MET:HE3	1:D:149:LEU:HD12	1.82	0.60
1:A:217:PHE:O	1:A:218:PHE:HB2	2.01	0.60
1:D:224:THR:CA	1:D:225:PRO:CB	2.79	0.60
1:D:124:ILE:HD11	1:D:207:ILE:HG23	1.84	0.60
1:D:72:THR:HG22	1:D:75:ASP:H	1.68	0.58
1:D:141:MET:CE	1:D:149:LEU:HD12	2.32	0.58
1:A:94:HIS:HD2	1:A:141:MET:CE	2.17	0.57
1:A:210:LYS:HE3	1:B:209:LEU:HD13	1.86	0.56
1:A:173:GLU:OE1	1:B:196:LYS:NZ	2.37	0.56
1:A:94:HIS:HD2	1:A:141:MET:HE2	1.70	0.56
1:B:180:GLU:O	1:B:183:THR:HG22	2.06	0.54
1:D:84:TRP:CD1	1:D:85:ASN:N	2.76	0.54
1:D:141:MET:HE2	1:D:146:LEU:HA	1.90	0.53
1:D:25:GLU:N	1:D:26:PRO:HA	2.23	0.53
1:C:141:MET:HE3	1:C:146:LEU:HB2	1.91	0.51
1:B:223:ASP:O	1:B:225:PRO:HD3	2.12	0.50
1:A:94:HIS:CD2	1:A:141:MET:CE	2.95	0.50
1:B:141:MET:HE3	1:B:146:LEU:HB2	1.94	0.50
1:A:54:GLN:C	1:A:56:PHE:H	2.15	0.49
1:B:113:ARG:HG2	1:B:117:HIS:HD2	1.77	0.49
1:A:219:LYS:CB	1:A:220:LEU:HB2	2.43	0.49
1:C:105:LEU:HB2	1:C:109:LEU:HB2	1.94	0.49
1:A:94:HIS:CD2	1:A:141:MET:HE3	2.48	0.49
1:B:225:PRO:HG2	1:D:59:VAL:HG21	1.95	0.48
1:A:18:LEU:HD22	1:A:22:LEU:HG	1.96	0.48
1:D:81:ARG:HA	1:D:84:TRP:HE3	1.79	0.47
1:D:141:MET:HE2	1:D:146:LEU:CA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:O	1:A:183:THR:HB	2.15	0.47
1:A:55:LEU:HD22	1:A:88:LEU:HD11	1.96	0.46
1:C:125:PHE:CE1	1:C:129:LEU:HD11	2.49	0.46
1:C:189:GLU:O	1:C:191:PRO:HD3	2.15	0.46
1:A:180:GLU:O	1:A:184:LYS:HG3	2.16	0.46
1:B:16:ARG:HD3	1:B:66:PRO:HG3	1.98	0.46
1:B:164:ASN:ND2	1:B:167:GLU:CB	2.79	0.46
1:A:183:THR:HG21	1:A:194:PHE:HB2	1.97	0.46
1:B:113:ARG:HG2	1:B:117:HIS:CD2	2.50	0.46
1:C:113:ARG:HG2	1:C:117:HIS:HD2	1.81	0.45
1:A:21:GLU:OE2	1:A:147:GLY:HA2	2.16	0.45
1:D:85:ASN:ND2	1:D:208:GLY:O	2.49	0.45
1:B:164:ASN:HD22	1:B:167:GLU:CB	2.29	0.45
1:A:219:LYS:HA	1:A:220:LEU:CG	2.45	0.45
1:A:58:LEU:HD11	1:A:87:LEU:HD13	1.98	0.45
1:C:85:ASN:HD21	1:C:211:CYS:HB2	1.82	0.45
1:B:61:TRP:CZ3	1:B:154:LEU:HD22	2.52	0.45
1:C:54:GLN:C	1:C:56:PHE:H	2.21	0.44
1:A:105:LEU:O	1:A:107:THR:N	2.50	0.44
1:A:124:ILE:HD13	1:A:210:LYS:HB3	2.00	0.43
1:A:210:LYS:N	1:A:210:LYS:HE2	2.33	0.43
1:C:215:LEU:HD13	1:C:216:PHE:H	1.83	0.43
1:B:179:LEU:HD11	1:B:197:LEU:HD13	1.99	0.43
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.79	0.43
1:A:59:VAL:HG12	1:A:63:LYS:HD2	2.00	0.43
1:A:72:THR:HG23	1:A:74:GLU:OE2	2.18	0.43
1:A:95:ARG:CZ	1:A:106:ALA:HB2	2.49	0.43
1:B:129:LEU:HA	1:B:133:VAL:HB	2.01	0.43
1:C:127:ARG:NH1	1:C:210:LYS:HD3	2.34	0.42
1:C:85:ASN:ND2	1:C:208:GLY:O	2.53	0.42
1:C:214:HIS:O	1:C:215:LEU:O	2.38	0.42
1:D:80:LEU:O	1:D:84:TRP:HB3	2.18	0.42
1:D:211:CYS:C	1:D:213:GLU:H	2.23	0.41
1:D:213:GLU:O	1:D:214:HIS:HB2	2.20	0.41
1:C:215:LEU:HD13	1:C:216:PHE:N	2.35	0.41
1:D:12:MET:O	1:D:178:THR:HG21	2.20	0.41
1:A:141:MET:HE3	1:A:146:LEU:HB2	2.02	0.41
1:C:225:PRO:C	1:C:227:ASP:H	2.24	0.40
1:A:92:PHE:C	1:A:92:PHE:CD1	2.94	0.40
1:D:107:THR:OG1	1:D:109:LEU:HB2	2.21	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	186/241 (77%)	169 (91%)	9 (5%)	8 (4%)	2	2
1	B	188/241 (78%)	168 (89%)	13 (7%)	7 (4%)	3	2
1	C	190/241 (79%)	170 (90%)	8 (4%)	12 (6%)	1	0
1	D	191/241 (79%)	178 (93%)	7 (4%)	6 (3%)	4	3
All	All	755/964 (78%)	685 (91%)	37 (5%)	33 (4%)	2	2

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	218	PHE
1	A	220	LEU
1	B	51	ALA
1	B	53	LYS
1	B	221	ILE
1	C	52	ASP
1	C	54	GLN
1	C	215	LEU
1	D	225	PRO
1	D	227	ASP
1	A	51	ALA
1	A	53	LYS
1	A	106	ALA
1	B	55	LEU
1	B	215	LEU
1	B	220	LEU
1	C	51	ALA
1	C	55	LEU
1	C	219	LYS
1	D	220	LEU
1	D	221	ILE

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Mol	Chain	Res	Type
1	C	101	ASP
1	C	109	LEU
1	C	220	LEU
1	C	225	PRO
1	D	212	LEU
1	D	214	HIS
1	C	214	HIS
1	C	221	ILE
1	A	216	PHE
1	B	99	VAL
1	A	221	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	155/211 (74%)	141 (91%)	14 (9%)	9	14
1	B	151/211 (72%)	137 (91%)	14 (9%)	9	13
1	C	150/211 (71%)	139 (93%)	11 (7%)	14	22
1	D	149/211 (71%)	136 (91%)	13 (9%)	10	15
All	All	605/844 (72%)	553 (91%)	52 (9%)	10	16

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	18	LEU
1	A	69	SER
1	A	72	THR
1	A	81	ARG
1	A	92	PHE
1	A	104	LEU
1	A	113	ARG
1	A	160	LYS
1	A	176	TYR

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Mol	Chain	Res	Type
1	A	183	THR
1	A	210	LYS
1	A	216	PHE
1	A	224	THR
1	B	11	ASP
1	B	14	VAL
1	B	15	GLU
1	B	18	LEU
1	B	56	PHE
1	B	57	THR
1	B	70	ASP
1	B	104	LEU
1	B	114	SER
1	B	160	LYS
1	B	169	GLU
1	B	176	TYR
1	B	183	THR
1	B	210	LYS
1	C	11	ASP
1	C	14	VAL
1	C	18	LEU
1	C	25	GLU
1	C	57	THR
1	C	84	TRP
1	C	88	LEU
1	C	104	LEU
1	C	189	GLU
1	C	210	LYS
1	C	214	HIS
1	D	14	VAL
1	D	18	LEU
1	D	72	THR
1	D	84	TRP
1	D	92	PHE
1	D	100	GLN
1	D	109	LEU
1	D	143	LYS
1	D	160	LYS
1	D	206	SER
1	D	210	LYS
1	D	214	HIS
1	D	215	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	110	HIS
1	B	85	ASN
1	B	100	GLN
1	B	117	HIS
1	B	164	ASN
1	C	85	ASN
1	C	117	HIS
1	D	112	HIS

### 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	190/241 (78%)	0.52	14 (7%) 14 13	41, 54, 74, 86	0
1	B	192/241 (79%)	0.32	9 (4%) 31 30	44, 63, 84, 87	0
1	C	194/241 (80%)	0.50	10 (5%) 27 26	43, 62, 75, 78	0
1	D	195/241 (80%)	0.63	11 (5%) 24 23	45, 69, 91, 95	0
All	All	771/964 (79%)	0.49	44 (5%) 23 22	41, 62, 85, 95	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	ALA	13.4
1	D	26	PRO	7.2
1	D	107	THR	6.5
1	C	218	PHE	6.1
1	A	107	THR	6.0
1	A	101	ASP	4.7
1	A	102	GLY	4.5
1	A	218	PHE	4.5
1	C	26	PRO	4.5
1	A	80	LEU	3.7
1	A	103	ILE	3.5
1	A	213	GLU	3.3
1	A	215	LEU	3.0
1	C	162	LEU	2.9
1	A	106	ALA	2.9
1	C	75	ASP	2.7
1	D	187	TYR	2.7
1	D	213	GLU	2.6
1	B	214	HIS	2.6
1	C	59	VAL	2.6
1	B	215	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	111	VAL	2.6
1	B	106	ALA	2.6
1	C	216	PHE	2.6
1	A	212	LEU	2.5
1	D	220	LEU	2.5
1	B	217	PHE	2.5
1	B	175	VAL	2.3
1	C	214	HIS	2.3
1	A	109	LEU	2.3
1	B	73	LEU	2.3
1	B	212	LEU	2.2
1	C	215	LEU	2.2
1	D	11	ASP	2.1
1	D	88	LEU	2.1
1	D	92	PHE	2.1
1	D	215	LEU	2.1
1	C	224	THR	2.1
1	C	220	LEU	2.1
1	A	126	ASP	2.1
1	D	81	ARG	2.1
1	B	216	PHE	2.0
1	B	107	THR	2.0
1	A	209	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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.