



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 2QW4 / pdb_00002qw4
Title : Human NR4A1 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 : 2007-08-09
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

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

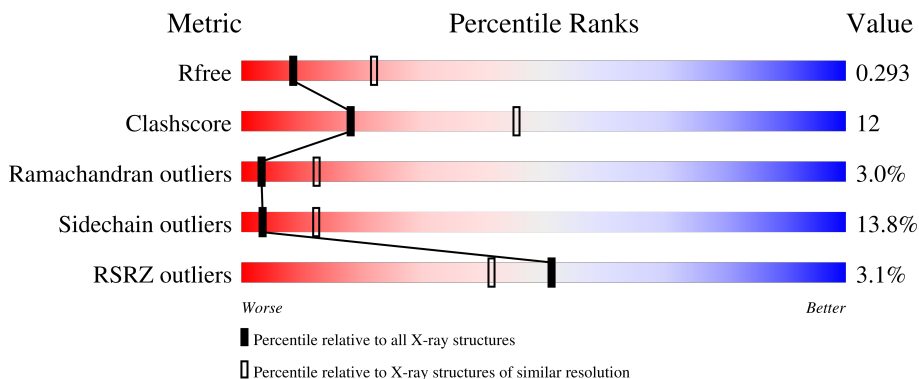
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	273	2% 54% 25% • • 16%
1	B	273	3% 55% 24% 5% • 16%
1	C	273	3% 58% 21% • 17%
1	D	273	3% 54% 25% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7147 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 Orphan nuclear receptor NR4A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1781	1145	307	323	6			
1	B	230	Total	C	N	O	S	0	0	0
			1793	1155	307	324	7			
1	C	227	Total	C	N	O	S	0	0	0
			1777	1149	302	319	7			
1	D	227	Total	C	N	O	S	0	0	0
			1786	1152	305	322	7			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P22736
A	-4	GLY	-	expression tag	UNP P22736
A	-3	SER	-	expression tag	UNP P22736
A	-2	SER	-	expression tag	UNP P22736
A	-1	HIS	-	expression tag	UNP P22736
A	0	HIS	-	expression tag	UNP P22736
A	1	HIS	-	expression tag	UNP P22736
A	2	HIS	-	expression tag	UNP P22736
A	3	HIS	-	expression tag	UNP P22736
A	4	HIS	-	expression tag	UNP P22736
A	5	SER	-	expression tag	UNP P22736
A	6	SER	-	expression tag	UNP P22736
A	7	GLY	-	expression tag	UNP P22736
A	8	LEU	-	expression tag	UNP P22736
A	9	VAL	-	expression tag	UNP P22736
A	10	PRO	-	expression tag	UNP P22736
A	11	ARG	-	expression tag	UNP P22736
A	12	GLY	-	expression tag	UNP P22736
A	13	SER	-	expression tag	UNP P22736
A	14	HIS	-	expression tag	UNP P22736
A	15	MET	-	expression tag	UNP P22736

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	expression tag	UNP P22736
B	-4	GLY	-	expression tag	UNP P22736
B	-3	SER	-	expression tag	UNP P22736
B	-2	SER	-	expression tag	UNP P22736
B	-1	HIS	-	expression tag	UNP P22736
B	0	HIS	-	expression tag	UNP P22736
B	1	HIS	-	expression tag	UNP P22736
B	2	HIS	-	expression tag	UNP P22736
B	3	HIS	-	expression tag	UNP P22736
B	4	HIS	-	expression tag	UNP P22736
B	5	SER	-	expression tag	UNP P22736
B	6	SER	-	expression tag	UNP P22736
B	7	GLY	-	expression tag	UNP P22736
B	8	LEU	-	expression tag	UNP P22736
B	9	VAL	-	expression tag	UNP P22736
B	10	PRO	-	expression tag	UNP P22736
B	11	ARG	-	expression tag	UNP P22736
B	12	GLY	-	expression tag	UNP P22736
B	13	SER	-	expression tag	UNP P22736
B	14	HIS	-	expression tag	UNP P22736
B	15	MET	-	expression tag	UNP P22736
C	-5	MET	-	expression tag	UNP P22736
C	-4	GLY	-	expression tag	UNP P22736
C	-3	SER	-	expression tag	UNP P22736
C	-2	SER	-	expression tag	UNP P22736
C	-1	HIS	-	expression tag	UNP P22736
C	0	HIS	-	expression tag	UNP P22736
C	1	HIS	-	expression tag	UNP P22736
C	2	HIS	-	expression tag	UNP P22736
C	3	HIS	-	expression tag	UNP P22736
C	4	HIS	-	expression tag	UNP P22736
C	5	SER	-	expression tag	UNP P22736
C	6	SER	-	expression tag	UNP P22736
C	7	GLY	-	expression tag	UNP P22736
C	8	LEU	-	expression tag	UNP P22736
C	9	VAL	-	expression tag	UNP P22736
C	10	PRO	-	expression tag	UNP P22736
C	11	ARG	-	expression tag	UNP P22736
C	12	GLY	-	expression tag	UNP P22736
C	13	SER	-	expression tag	UNP P22736
C	14	HIS	-	expression tag	UNP P22736
C	15	MET	-	expression tag	UNP P22736

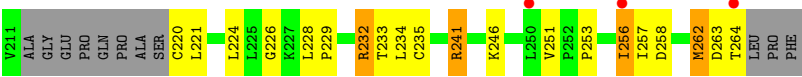
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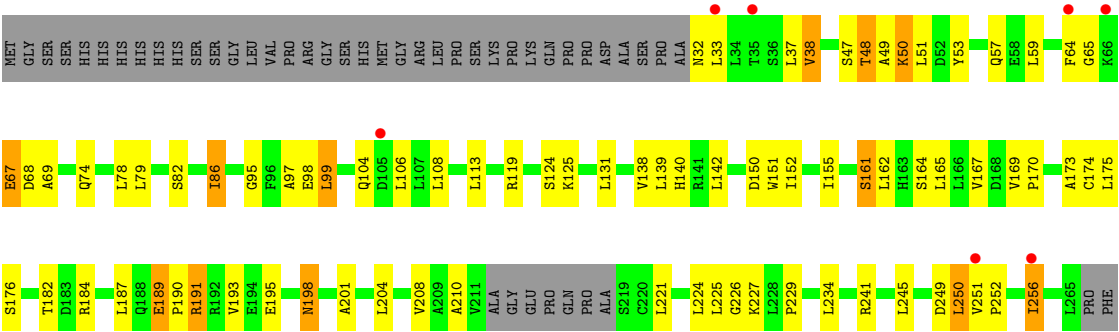
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	expression tag	UNP P22736
D	-4	GLY	-	expression tag	UNP P22736
D	-3	SER	-	expression tag	UNP P22736
D	-2	SER	-	expression tag	UNP P22736
D	-1	HIS	-	expression tag	UNP P22736
D	0	HIS	-	expression tag	UNP P22736
D	1	HIS	-	expression tag	UNP P22736
D	2	HIS	-	expression tag	UNP P22736
D	3	HIS	-	expression tag	UNP P22736
D	4	HIS	-	expression tag	UNP P22736
D	5	SER	-	expression tag	UNP P22736
D	6	SER	-	expression tag	UNP P22736
D	7	GLY	-	expression tag	UNP P22736
D	8	LEU	-	expression tag	UNP P22736
D	9	VAL	-	expression tag	UNP P22736
D	10	PRO	-	expression tag	UNP P22736
D	11	ARG	-	expression tag	UNP P22736
D	12	GLY	-	expression tag	UNP P22736
D	13	SER	-	expression tag	UNP P22736
D	14	HIS	-	expression tag	UNP P22736
D	15	MET	-	expression tag	UNP P22736

- Molecule 2 is water.

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



● Molecule 1: Orphan nuclear receptor NR4A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.53Å 96.36Å 144.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.80 48.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.17-2.80) 98.5 (48.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.292 0.227 , 0.293	Depositor DCC
R_{free} test set	1566 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7147	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.92	4/1816 (0.2%)	1.14	8/2457 (0.3%)
1	B	0.91	2/1829 (0.1%)	1.20	10/2475 (0.4%)
1	C	0.88	2/1814 (0.1%)	1.07	0/2455
1	D	0.75	1/1822 (0.1%)	1.08	5/2465 (0.2%)
All	All	0.87	9/7281 (0.1%)	1.13	23/9852 (0.2%)

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	1
1	C	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	PRO	N-CA	13.54	1.67	1.47
1	A	217	PRO	CA-CB	-8.13	1.37	1.53
1	A	191	ARG	CZ-NH2	-7.57	1.23	1.33
1	A	191	ARG	NE-CZ	-6.67	1.25	1.33
1	C	74	GLN	CB-CG	6.48	1.71	1.52
1	B	217	PRO	CA-CB	6.19	1.65	1.53
1	A	217	PRO	CA-C	-6.14	1.40	1.52
1	C	74	GLN	N-CA	5.25	1.52	1.46
1	D	256	ILE	CA-CB	5.21	1.60	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	PRO	N-CA-CB	19.97	124.97	103.00
1	B	50	LYS	N-CA-C	10.12	122.81	108.54
1	A	191	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	A	217	PRO	N-CA-C	-6.91	94.83	112.10
1	A	191	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	A	143	GLN	N-CA-C	-6.50	104.28	111.82
1	A	220	CYS	N-CA-C	6.09	128.06	111.00
1	B	49	ALA	CA-C-N	-5.86	115.11	123.20
1	B	49	ALA	C-N-CA	-5.86	115.11	123.20
1	B	217	PRO	N-CA-C	-5.80	97.61	112.10
1	B	169	VAL	CA-C-N	-5.79	112.95	118.97
1	B	169	VAL	C-N-CA	-5.79	112.95	118.97
1	A	217	PRO	N-CA-CB	5.78	109.36	103.00
1	B	251	VAL	N-CA-CB	5.55	115.71	109.99
1	A	60	VAL	N-CA-C	-5.23	107.62	112.43
1	D	198	ASN	N-CA-C	5.21	116.96	111.28
1	B	254	PRO	CA-C-N	5.19	126.33	119.84
1	B	254	PRO	C-N-CA	5.19	126.33	119.84
1	D	189	GLU	CA-C-N	5.19	124.50	118.85
1	D	189	GLU	C-N-CA	5.19	124.50	118.85
1	D	65	GLY	N-CA-C	5.14	119.57	112.52
1	D	161	SER	N-CA-C	5.12	117.25	111.11
1	A	253	PRO	O-C-N	5.05	123.52	121.15

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	SER	Peptide
1	B	50	LYS	Peptide
1	C	30	PRO	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	1781	0	1805	49	0
1	B	1793	0	1821	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1777	0	1819	32	0
1	D	1786	0	1827	40	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
All	All	7147	0	7272	175	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 (175) 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:C:117:ILE:HD12	1:C:235:CYS:SG	1.91	1.10
1:B:221:LEU:H	1:B:221:LEU:HD23	1.20	1.05
1:C:184:ARG:HH12	1:C:232:ARG:HH12	1.05	1.02
1:B:146:ARG:HH11	1:B:146:ARG:HG2	1.26	0.98
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.37	0.90
1:B:91:GLU:OE2	1:B:91:GLU:HA	1.73	0.87
1:D:161:SER:OG	1:D:227:LYS:HE3	1.76	0.86
1:B:140:HIS:HD2	1:B:142:LEU:H	1.25	0.82
1:B:168:ASP:OD1	1:B:170:PRO:HD2	1.82	0.78
1:A:191:ARG:HD3	1:A:191:ARG:H	1.46	0.78
1:B:131:LEU:HD22	1:B:152:ILE:HD11	1.67	0.74
1:A:140:HIS:HD2	1:A:142:LEU:H	1.36	0.73
1:A:246:LYS:HE3	1:A:258:ASP:OD1	1.89	0.72
1:B:221:LEU:HD23	1:B:221:LEU:N	2.03	0.71
1:B:146:ARG:HG2	1:B:146:ARG:NH1	1.96	0.70
1:B:192:ARG:HH21	1:B:192:ARG:HG3	1.55	0.70
1:C:117:ILE:CD1	1:C:235:CYS:SG	2.75	0.70
1:C:184:ARG:HH12	1:C:232:ARG:NH1	1.86	0.69
1:B:221:LEU:H	1:B:221:LEU:CD2	2.00	0.68
1:C:184:ARG:NH1	1:C:232:ARG:HH12	1.87	0.68
1:D:67:GLU:H	1:D:67:GLU:CD	1.99	0.67
1:A:219:SER:HA	1:A:221:LEU:H	1.59	0.67
1:D:161:SER:OG	1:D:227:LYS:CE	2.43	0.66
1:C:140:HIS:CD2	1:C:142:LEU:H	2.15	0.66
1:A:220:CYS:H	1:A:223:ARG:NH2	1.94	0.65
1:D:82:SER:O	1:D:86:ILE:HD13	1.96	0.65
1:D:38:VAL:HG22	1:D:170:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ILE:HD11	1:D:119:ARG:HD3	1.78	0.64
1:B:192:ARG:HG3	1:B:192:ARG:NH2	2.10	0.64
1:B:209:ALA:C	1:B:211:VAL:H	2.06	0.64
1:A:51:LEU:HD13	1:A:53:TYR:HE1	1.64	0.63
1:C:140:HIS:HD2	1:C:142:LEU:H	1.45	0.62
1:A:72:VAL:HG12	1:A:76:TYR:CE2	2.34	0.62
1:A:222:SER:HA	1:A:225:LEU:HB2	1.81	0.62
1:A:226:GLY:O	1:A:229:PRO:HD2	2.00	0.62
1:A:84:GLU:HG2	1:A:88:LYS:HE3	1.81	0.61
1:A:191:ARG:NH2	1:A:191:ARG:HB2	2.16	0.61
1:A:131:LEU:HD22	1:A:152:ILE:HD11	1.84	0.60
1:A:206:GLU:O	1:A:209:ALA:HB3	2.02	0.60
1:D:191:ARG:O	1:D:195:GLU:HB2	2.01	0.60
1:B:46:PRO:HG3	1:B:134:CYS:O	2.02	0.59
1:A:219:SER:HA	1:A:221:LEU:N	2.16	0.59
1:A:96:PHE:CE2	1:A:104:GLN:HG2	2.38	0.59
1:A:191:ARG:HH21	1:A:191:ARG:N	2.01	0.58
1:D:189:GLU:HB3	1:D:191:ARG:HH22	1.68	0.58
1:B:209:ALA:O	1:B:211:VAL:N	2.34	0.58
1:C:187:LEU:O	1:C:190:PRO:HD3	2.05	0.57
1:A:158:PHE:O	1:A:161:SER:HB3	2.04	0.57
1:A:191:ARG:NH2	1:A:191:ARG:CB	2.67	0.57
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.15	0.57
1:C:168:ASP:OD1	1:C:170:PRO:HD2	2.04	0.57
1:C:124:SER:O	1:C:126:PRO:HD3	2.05	0.57
1:A:220:CYS:H	1:A:223:ARG:HH21	1.53	0.56
1:B:192:ARG:HH21	1:B:192:ARG:CG	2.19	0.56
1:D:170:PRO:O	1:D:173:ALA:HB3	2.06	0.56
1:A:233:THR:O	1:A:236:THR:HB	2.05	0.56
1:D:140:HIS:CD2	1:D:142:LEU:H	2.24	0.55
1:D:97:ALA:HA	1:D:104:GLN:NE2	2.21	0.55
1:C:79:LEU:HD23	1:C:257:ILE:HG21	1.89	0.55
1:A:191:ARG:H	1:A:191:ARG:HH21	1.55	0.55
1:A:90:ALA:HA	1:A:93:ILE:HD12	1.88	0.55
1:D:165:LEU:HB3	1:D:167:VAL:HG23	1.88	0.54
1:C:117:ILE:HD12	1:C:235:CYS:HG	1.72	0.54
1:A:191:ARG:HH21	1:A:191:ARG:CB	2.21	0.53
1:B:146:ARG:HH11	1:B:146:ARG:CG	2.11	0.53
1:D:226:GLY:O	1:D:229:PRO:HD2	2.09	0.53
1:B:91:GLU:OE2	1:B:91:GLU:CA	2.48	0.53
1:B:97:ALA:HA	1:B:104:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD21	1:D:193:VAL:HG22	1.91	0.53
1:A:258:ASP:O	1:A:262:MET:HG2	2.10	0.52
1:B:140:HIS:CD2	1:B:142:LEU:H	2.15	0.52
1:B:82:SER:O	1:B:86:ILE:HG13	2.09	0.52
1:D:187:LEU:HD13	1:D:193:VAL:HG21	1.92	0.52
1:B:67:GLU:H	1:B:67:GLU:CD	2.13	0.52
1:A:60:VAL:HG12	1:A:60:VAL:O	2.09	0.51
1:A:60:VAL:O	1:A:62:PRO:HD3	2.09	0.51
1:B:228:LEU:N	1:B:229:PRO:HD2	2.26	0.51
1:D:131:LEU:HD22	1:D:152:ILE:HD11	1.93	0.51
1:A:106:LEU:HD23	1:A:187:LEU:HD23	1.91	0.51
1:B:47:SER:OG	1:B:49:ALA:HB3	2.10	0.51
1:D:162:LEU:O	1:D:165:LEU:HB2	2.11	0.51
1:B:141:ARG:HB3	1:B:141:ARG:NH1	2.26	0.50
1:A:63:HIS:HD2	1:A:146:ARG:HH21	1.60	0.50
1:B:108:LEU:HD13	1:B:180:LEU:HD11	1.93	0.50
1:B:97:ALA:HA	1:B:104:GLN:NE2	2.26	0.50
1:A:247:LEU:C	1:A:249:ASP:N	2.69	0.50
1:C:72:VAL:HG12	1:C:251:VAL:HG22	1.92	0.50
1:D:140:HIS:HD2	1:D:142:LEU:H	1.59	0.50
1:B:63:HIS:HB3	1:B:146:ARG:HH21	1.75	0.50
1:A:72:VAL:HG12	1:A:76:TYR:HE2	1.78	0.49
1:B:227:LYS:HA	1:B:227:LYS:HE2	1.93	0.49
1:C:123:ARG:NH2	1:C:134:CYS:HB3	2.27	0.48
1:D:198:ASN:O	1:D:201:ALA:HB3	2.13	0.48
1:B:242:ILE:O	1:B:243:PHE:C	2.56	0.48
1:C:50:LYS:HA	1:C:50:LYS:HE3	1.95	0.48
1:C:131:LEU:HD22	1:C:152:ILE:HD11	1.94	0.48
1:A:219:SER:HB2	1:A:222:SER:H	1.78	0.47
1:A:114:GLU:HG2	1:A:235:CYS:SG	2.55	0.47
1:D:95:GLY:O	1:D:98:GLU:HB2	2.15	0.47
1:A:160:ARG:CZ	1:A:160:ARG:HB2	2.45	0.47
1:B:74:GLN:O	1:B:78:LEU:HD22	2.15	0.47
1:C:131:LEU:HD13	1:C:144:CYS:SG	2.54	0.47
1:B:147:GLY:O	1:B:241:ARG:NH1	2.48	0.46
1:C:168:ASP:CG	1:C:170:PRO:HD2	2.40	0.46
1:B:121:ALA:HA	1:B:159:SER:HB2	1.97	0.46
1:C:199:ARG:O	1:C:203:CYS:HB3	2.15	0.46
1:B:33:LEU:HD23	1:B:203:CYS:SG	2.55	0.46
1:C:154:SER:HB3	1:C:234:LEU:CD1	2.45	0.46
1:D:208:VAL:HG21	1:D:221:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:HG12	1:B:138:VAL:HG22	1.97	0.46
1:D:33:LEU:O	1:D:37:LEU:N	2.38	0.46
1:D:124:SER:C	1:D:125:LYS:HG2	2.41	0.46
1:D:189:GLU:CB	1:D:191:ARG:HH22	2.29	0.46
1:C:241:ARG:HD2	1:C:241:ARG:O	2.16	0.45
1:B:77:ASP:O	1:B:78:LEU:C	2.58	0.45
1:C:228:LEU:HB2	1:C:229:PRO:HD3	1.98	0.45
1:D:249:ASP:O	1:D:250:LEU:C	2.59	0.45
1:D:47:SER:H	1:D:50:LYS:HD2	1.82	0.45
1:A:140:HIS:CD2	1:A:142:LEU:H	2.26	0.45
1:B:61:LEU:HD13	1:D:225:LEU:HD11	1.98	0.45
1:C:226:GLY:O	1:C:229:PRO:HD2	2.17	0.45
1:A:200:ILE:O	1:A:203:CYS:HB3	2.17	0.45
1:B:117:ILE:HD13	1:B:234:LEU:HB3	1.99	0.45
1:B:99:LEU:HD23	1:B:192:ARG:NH2	2.32	0.44
1:C:168:ASP:OD1	1:C:168:ASP:C	2.60	0.44
1:C:151:TRP:O	1:C:154:SER:HB2	2.18	0.44
1:D:169:VAL:HB	1:D:170:PRO:HD3	1.98	0.44
1:A:63:HIS:CD2	1:A:146:ARG:NH2	2.85	0.44
1:B:53:TYR:O	1:B:55:LYS:N	2.50	0.44
1:D:69:ALA:HB1	1:D:251:VAL:HG13	1.99	0.44
1:A:66:LYS:O	1:A:67:GLU:C	2.60	0.44
1:A:126:PRO:C	1:A:128:GLU:H	2.25	0.44
1:B:123:ARG:HG3	1:B:132:ILE:HB	1.99	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.94	0.43
1:B:50:LYS:HA	1:B:50:LYS:HD3	1.61	0.43
1:C:229:PRO:O	1:C:233:THR:HG23	2.19	0.43
1:A:104:GLN:O	1:A:108:LEU:HB2	2.18	0.43
1:C:202:SER:HA	1:C:205:LYS:HB2	2.01	0.43
1:D:204:LEU:HG	1:D:221:LEU:HD11	2.01	0.43
1:D:251:VAL:HA	1:D:252:PRO:HD3	1.91	0.43
1:C:82:SER:O	1:C:83:LEU:C	2.61	0.43
1:A:169:VAL:O	1:A:170:PRO:C	2.60	0.43
1:C:34:LEU:HD11	1:C:170:PRO:HB3	1.99	0.43
1:C:256:ILE:H	1:C:256:ILE:HG13	1.67	0.43
1:D:32:ASN:HB3	1:D:33:LEU:H	1.63	0.42
1:B:88:LYS:O	1:B:91:GLU:HB3	2.19	0.42
1:D:48:THR:HA	1:D:51:LEU:HG	2.00	0.42
1:B:243:PHE:HD1	1:B:261:PHE:HZ	1.67	0.42
1:D:74:GLN:O	1:D:78:LEU:HB2	2.19	0.42
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:O	1:A:163:HIS:HE1	2.02	0.42
1:A:35:THR:O	1:A:36:SER:C	2.62	0.42
1:B:229:PRO:O	1:B:232:ARG:N	2.44	0.42
1:A:227:LYS:HA	1:A:227:LYS:HE2	2.01	0.41
1:B:93:ILE:HA	1:B:94:PRO:HD2	1.90	0.41
1:D:151:TRP:CE2	1:D:155:ILE:HD11	2.55	0.41
1:D:184:ARG:H	1:D:187:LEU:HD12	1.85	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.68	0.41
1:B:53:TYR:C	1:B:55:LYS:N	2.79	0.41
1:D:67:GLU:CD	1:D:67:GLU:N	2.76	0.41
1:B:229:PRO:O	1:B:232:ARG:HB2	2.20	0.41
1:C:253:PRO:HG2	1:C:258:ASP:OD2	2.21	0.41
1:B:141:ARG:HH11	1:B:141:ARG:CB	2.34	0.41
1:A:89:TRP:CZ2	1:A:93:ILE:HD11	2.56	0.41
1:A:161:SER:OG	1:A:227:LYS:NZ	2.54	0.41
1:B:53:TYR:C	1:B:55:LYS:H	2.29	0.41
1:B:141:ARG:NH1	1:B:141:ARG:CB	2.84	0.41
1:B:254:PRO:HA	1:B:255:PRO:HD2	1.81	0.41
1:D:53:TYR:CE1	1:D:138:VAL:HG21	2.56	0.40
1:D:190:PRO:O	1:D:193:VAL:HB	2.21	0.40
1:A:63:HIS:HD2	1:A:146:ARG:NH2	2.19	0.40
1:D:241:ARG:O	1:D:245:LEU:HG	2.20	0.40
1:A:36:SER:HB2	1:A:94:PRO:HG2	2.04	0.40
1:A:51:LEU:HD13	1:A:53:TYR:CE1	2.50	0.40
1:C:151:TRP:O	1:C:154:SER:N	2.55	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	226/273 (83%)	204 (90%)	17 (8%)	5 (2%)	5 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	226/273 (83%)	201 (89%)	15 (7%)	10 (4%)	2	7
1	C	223/273 (82%)	190 (85%)	27 (12%)	6 (3%)	4	15
1	D	223/273 (82%)	205 (92%)	12 (5%)	6 (3%)	4	15
All	All	898/1092 (82%)	800 (89%)	71 (8%)	27 (3%)	3	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ALA
1	A	212	ALA
1	A	250	LEU
1	B	211	VAL
1	C	31	ALA
1	C	141	ARG
1	D	250	LEU
1	B	210	ALA
1	B	219	SER
1	D	49	ALA
1	D	150	ASP
1	B	250	LEU
1	C	50	LYS
1	C	262	MET
1	C	263	ASP
1	D	210	ALA
1	B	43	ASP
1	B	263	ASP
1	C	52	ASP
1	D	57	GLN
1	A	67	GLU
1	A	220	CYS
1	B	49	ALA
1	B	54	SER
1	B	224	LEU
1	B	255	PRO
1	D	38	VAL

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	193/235 (82%)	166 (86%)	27 (14%)	3	12
1	B	195/235 (83%)	170 (87%)	25 (13%)	4	15
1	C	195/235 (83%)	161 (83%)	34 (17%)	2	7
1	D	197/235 (84%)	175 (89%)	22 (11%)	6	19
All	All	780/940 (83%)	672 (86%)	108 (14%)	3	12

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	50	LYS
1	A	51	LEU
1	A	61	LEU
1	A	67	GLU
1	A	79	LEU
1	A	80	SER
1	A	88	LYS
1	A	91	GLU
1	A	98	GLU
1	A	114	GLU
1	A	123	ARG
1	A	125	LYS
1	A	128	GLU
1	A	132	ILE
1	A	146	ARG
1	A	154	SER
1	A	165	LEU
1	A	175	LEU
1	A	191	ARG
1	A	206	GLU
1	A	208	VAL
1	A	221	LEU
1	A	224	LEU
1	A	232	ARG
1	A	259	LYS
1	A	260	ILE
1	B	32	ASN
1	B	48	THR
1	B	50	LYS

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Mol	Chain	Res	Type
1	B	57	GLN
1	B	64	PHE
1	B	67	GLU
1	B	78	LEU
1	B	80	SER
1	B	91	GLU
1	B	98	GLU
1	B	100	SER
1	B	108	LEU
1	B	113	LEU
1	B	139	LEU
1	B	146	ARG
1	B	165	LEU
1	B	175	LEU
1	B	192	ARG
1	B	195	GLU
1	B	221	LEU
1	B	223	ARG
1	B	224	LEU
1	B	241	ARG
1	B	247	LEU
1	B	256	ILE
1	C	34	LEU
1	C	36	SER
1	C	50	LYS
1	C	55	LYS
1	C	74	GLN
1	C	78	LEU
1	C	79	LEU
1	C	82	SER
1	C	93	ILE
1	C	98	GLU
1	C	99	LEU
1	C	108	LEU
1	C	139	LEU
1	C	150	ASP
1	C	152	ILE
1	C	160	ARG
1	C	164	SER
1	C	166	LEU
1	C	169	VAL
1	C	175	LEU

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Mol	Chain	Res	Type
1	C	191	ARG
1	C	196	LEU
1	C	200	ILE
1	C	203	CYS
1	C	205	LYS
1	C	220	CYS
1	C	221	LEU
1	C	224	LEU
1	C	232	ARG
1	C	241	ARG
1	C	246	LYS
1	C	256	ILE
1	C	262	MET
1	C	264	THR
1	D	48	THR
1	D	50	LYS
1	D	59	LEU
1	D	64	PHE
1	D	67	GLU
1	D	68	ASP
1	D	79	LEU
1	D	86	ILE
1	D	99	LEU
1	D	106	LEU
1	D	108	LEU
1	D	113	LEU
1	D	139	LEU
1	D	164	SER
1	D	174	CYS
1	D	175	LEU
1	D	176	SER
1	D	182	THR
1	D	191	ARG
1	D	224	LEU
1	D	234	LEU
1	D	256	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	104	GLN

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Mol	Chain	Res	Type
1	A	140	HIS
1	B	73	GLN
1	B	104	GLN
1	B	140	HIS
1	B	207	HIS
1	C	57	GLN
1	C	63	HIS
1	C	74	GLN
1	C	140	HIS
1	C	197	GLN
1	C	237	GLN
1	C	240	GLN
1	D	140	HIS
1	D	188	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	230/273 (84%)	0.05	6 (2%) 57 47	30, 52, 72, 77	0
1	B	230/273 (84%)	0.13	7 (3%) 52 42	31, 51, 65, 74	0
1	C	227/273 (83%)	0.18	8 (3%) 47 38	38, 54, 72, 81	0
1	D	227/273 (83%)	0.30	7 (3%) 51 41	46, 62, 81, 85	0
All	All	914/1092 (83%)	0.16	28 (3%) 51 41	30, 54, 77, 85	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	PRO	5.7
1	B	62	PRO	5.1
1	C	74	GLN	4.9
1	C	264	THR	4.4
1	B	69	ALA	4.1
1	B	229	PRO	3.7
1	C	250	LEU	3.5
1	A	48	THR	3.4
1	A	217	PRO	3.2
1	B	63	HIS	3.2
1	D	35	THR	3.1
1	D	64	PHE	2.8
1	D	66	LYS	2.7
1	B	264	THR	2.7
1	A	61	LEU	2.7
1	D	33	LEU	2.6
1	C	49	ALA	2.5
1	C	256	ILE	2.5
1	D	256	ILE	2.5
1	A	213	GLY	2.4
1	C	77	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	150	ASP	2.3
1	C	51	LEU	2.3
1	A	62	PRO	2.3
1	A	264	THR	2.3
1	D	251	VAL	2.2
1	D	105	ASP	2.1
1	B	64	PHE	2.1

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 oligosaccharides 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.