



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:06 PM GMT

PDB ID : 2QW4
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

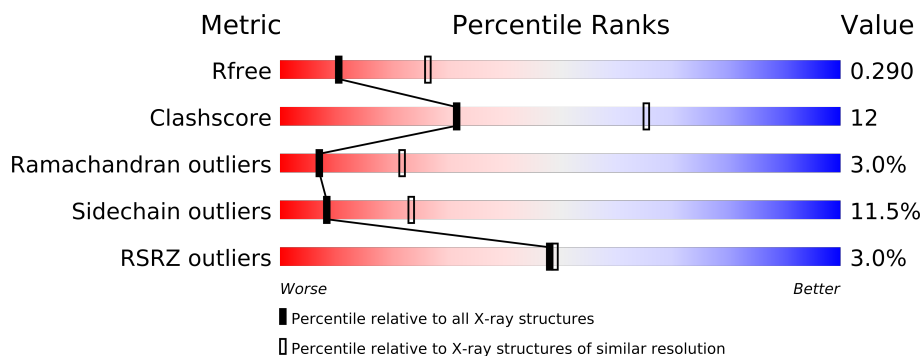
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7147 atoms, of which 0 are hydrogen and 0 are deuterium.

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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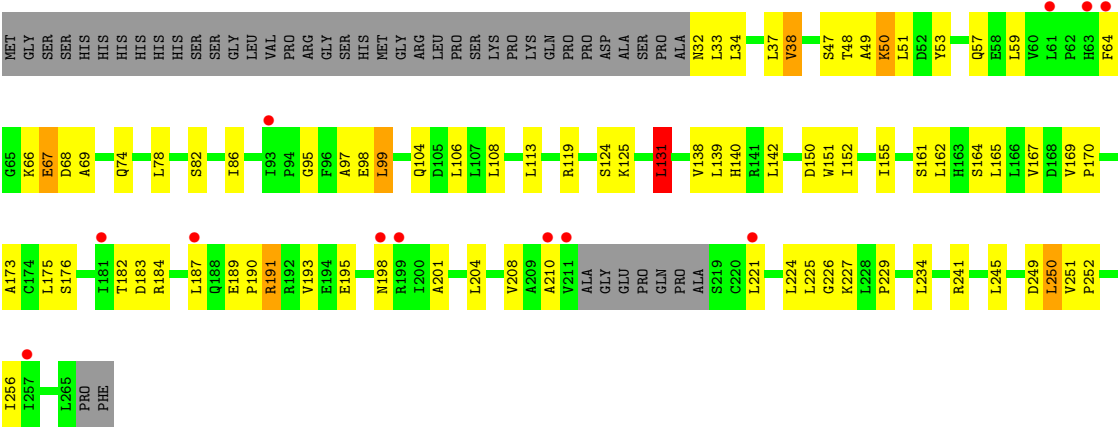
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	EXPRESSION TAG	UNP P22736
D	-4	GLY	-	EXPRESSION TAG	UNP P22736
D	-3	SER	-	EXPRESSION TAG	UNP P22736
D	-2	SER	-	EXPRESSION TAG	UNP P22736
D	-1	HIS	-	EXPRESSION TAG	UNP P22736
D	0	HIS	-	EXPRESSION TAG	UNP P22736
D	1	HIS	-	EXPRESSION TAG	UNP P22736
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

Chain D: 



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 48.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.17-2.80) 98.5 (48.18-2.80)	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 0.229 , 0.290	Depositor DCC
R_{free} test set	1566 reflections (5.33%)	DCC
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 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 30959 reflections (0.003%)	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.

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	0.76	5/1816 (0.3%)	0.93	5/2457 (0.2%)
1	B	0.78	2/1829 (0.1%)	0.89	2/2475 (0.1%)
1	C	0.73	2/1814 (0.1%)	0.79	1/2455 (0.0%)
1	D	0.63	0/1822	0.73	1/2465 (0.0%)
All	All	0.73	9/7281 (0.1%)	0.84	9/9852 (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	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	11.82	1.67	1.47
1	A	217	PRO	CA-CB	-8.18	1.37	1.53
1	A	191	ARG	CZ-NH2	-7.26	1.23	1.33
1	C	74	GLN	CB-CG	7.17	1.71	1.52
1	A	217	PRO	CA-C	-6.39	1.40	1.52
1	B	217	PRO	CA-CB	6.14	1.65	1.53
1	A	203	CYS	CB-SG	-5.85	1.72	1.81
1	A	191	ARG	NE-CZ	-5.65	1.25	1.33
1	C	203	CYS	CB-SG	-5.37	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	PRO	N-CA-CB	18.06	124.97	103.30
1	A	191	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	A	191	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	217	PRO	N-CA-C	-6.64	94.83	112.10
1	A	220	CYS	N-CA-C	6.32	128.06	111.00
1	B	217	PRO	N-CA-C	-5.57	97.61	112.10
1	D	131	LEU	CA-CB-CG	-5.49	102.67	115.30
1	C	131	LEU	CA-CB-CG	-5.29	103.14	115.30
1	A	217	PRO	N-CA-CB	5.05	109.36	103.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1781	0	1805	45	0
1	B	1793	0	1821	53	0
1	C	1777	0	1819	30	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	167	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (167) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HG2	1:B:146:ARG:HH11	1.26	0.98
1:B:223:ARG:HH11	1:B:223:ARG:HG3	1.37	0.90
1:B:91:GLU:HA	1:B:91:GLU:OE2	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:N	1:B:221:LEU:HD23	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: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
1:D:86:ILE:HD11	1:D:119:ARG:HD3	1.78	0.64
1:B:192:ARG:NH2	1:B:192:ARG:HG3	2.10	0.64
1:A:51:LEU:HD13	1:A:53:TYR:HE1	1.64	0.63
1:D:67:GLU:CD	1:D:67:GLU:H	1.99	0.63
1:C:140:HIS:HD2	1:C:142:LEU:H	1.45	0.62
1:A:222:SER:HA	1:A:225:LEU:HB2	1.81	0.62
1:A:72:VAL:HG12	1:A:76:TYR:CE2	2.34	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:C:117:ILE:HD12	1:C:235:CYS:HG	1.65	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:209:ALA:C	1:B:211:VAL:H	2.06	0.59
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:PHE:CE2	1:A:104:GLN:HG2	2.38	0.59
1:A:191:ARG:N	1:A:191:ARG:HH21	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:B:223:ARG:HH11	1:B:223:ARG:CG	2.15	0.57
1:A:191:ARG:NH2	1:A:191:ARG:CB	2.67	0.57
1:A:158:PHE:O	1:A:161:SER:HB3	2.04	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:CG	1:B:192:ARG:HH21	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:HH21	1:A:191:ARG:H	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: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:CA	1:B:91:GLU:OE2	2.48	0.53
1:B:97:ALA:HA	1:B:104:GLN:HE22	1.74	0.53
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:A:60:VAL:O	1:A:60:VAL:HG12	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:D:162:LEU:O	1:D:165:LEU:HB2	2.11	0.51
1:B:47:SER:OG	1:B:49:ALA:HB3	2.10	0.51
1:B:141:ARG:NH1	1:B:141:ARG:HB3	2.26	0.50
1:D:161:SER:HG	1:D:227:LYS:HE3	1.72	0.50
1:B:108:LEU:HD13	1:B:180:LEU:HD11	1.93	0.50
1:A:63:HIS:HD2	1:A:146:ARG:HH21	1.60	0.50
1:B:97:ALA:HA	1:B:104:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:140:HIS:HD2	1:D:142:LEU:H	1.59	0.50
1:C:72:VAL:HG12	1:C:251:VAL:HG22	1.92	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:HE2	1:B:227:LYS:HA	1.93	0.49
1:D:198:ASN:O	1:D:201:ALA:HB3	2.13	0.48
1:C:123:ARG:NH2	1:C:134:CYS:HB3	2.27	0.48
1:C:131:LEU:HD22	1:C:152:ILE:HD11	1.94	0.48
1:C:50:LYS:HA	1:C:50:LYS:HE3	1.95	0.48
1:A:219:SER:HB2	1:A:222:SER:H	1.78	0.47
1:B:67:GLU:CD	1:B:67:GLU:H	2.13	0.47
1:D:95:GLY:O	1:D:98:GLU:HB2	2.15	0.47
1:A:114:GLU:HG2	1:A:235:CYS:SG	2.55	0.47
1:C:131:LEU:HD13	1:C:144:CYS:SG	2.54	0.47
1:B:74:GLN:O	1:B:78:LEU:HD22	2.15	0.47
1:A:160:ARG:HB2	1:A:160:ARG:CZ	2.45	0.47
1:B:147:GLY:O	1:B:241:ARG:NH1	2.48	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
1:B:132:ILE:HG12	1:B:138:VAL:HG22	1.97	0.46
1:D:189:GLU:CB	1:D:191:ARG:HH22	2.29	0.46
1:D:33:LEU:O	1:D:37:LEU:N	2.38	0.46
1:C:241:ARG:O	1:C:241:ARG:HD2	2.16	0.45
1:C:228:LEU:HB2	1:C:229:PRO:HD3	1.98	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:C:226:GLY:O	1:C:229:PRO:HD2	2.17	0.45
1:A:247:LEU:C	1:A:249:ASP:N	2.69	0.45
1:B:61:LEU:HD13	1:D:225:LEU:HD11	1.98	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:D:169:VAL:HB	1:D:170:PRO:HD3	1.98	0.44
1:C:151:TRP:O	1:C:154:SER:HB2	2.18	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:B:123:ARG:HG3	1:B:132:ILE:HB	1.99	0.43
1:B:242:ILE:O	1:B:243:PHE:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:229:PRO:O	1:C:233:THR:HG23	2.19	0.43
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.94	0.43
1:B:50:LYS:HA	1:B:50:LYS:HD3	1.61	0.43
1:A:104:GLN:O	1:A:108:LEU:HB2	2.18	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:202:SER:HA	1:C:205:LYS:HB2	2.01	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:HA	1:B:108:LEU:HD12	1.75	0.42
1:A:122:TYR:O	1:A:163:HIS:HE1	2.02	0.42
1:C:168:ASP:CG	1:C:170:PRO:HD2	2.40	0.42
1:B:229:PRO:O	1:B:232:ARG:N	2.44	0.42
1:A:227:LYS:HE2	1:A:227:LYS:HA	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: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:CB	1:B:141:ARG:HH11	2.34	0.41
1:A:161:SER:OG	1:A:227:LYS:NZ	2.54	0.41
1:A:89:TRP:CZ2	1:A:93:ILE:HD11	2.56	0.41
1:D:124:SER:C	1:D:125:LYS:HG2	2.41	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:B:77:ASP:O	1:B:78:LEU:C	2.58	0.41
1:D:249:ASP:O	1:D:250:LEU:C	2.59	0.41
1:D:190:PRO:O	1:D:193:VAL:HB	2.21	0.40
1:D:53:TYR:CE1	1:D:138:VAL:HG21	2.56	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: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
1:A:36:SER:HB2	1:A:94:PRO:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/273 (83%)	204 (90%)	17 (8%)	5 (2%)	10	32
1	B	226/273 (83%)	201 (89%)	15 (7%)	10 (4%)	4	12
1	C	223/273 (82%)	190 (85%)	27 (12%)	6 (3%)	8	25
1	D	223/273 (82%)	205 (92%)	12 (5%)	6 (3%)	8	25
All	All	898/1092 (82%)	800 (89%)	71 (8%)	27 (3%)	7	22

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

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Mol	Chain	Res	Type
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%)	172 (89%)	21 (11%)	9	26
1	B	195/235 (83%)	172 (88%)	23 (12%)	8	22
1	C	195/235 (83%)	171 (88%)	24 (12%)	7	20
1	D	197/235 (84%)	175 (89%)	22 (11%)	9	25
All	All	780/940 (83%)	690 (88%)	90 (12%)	8	23

All (90) 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	103	ASP
1	A	114	GLU
1	A	123	ARG
1	A	125	LYS
1	A	128	GLU
1	A	146	ARG
1	A	154	SER
1	A	175	LEU
1	A	191	ARG
1	A	206	GLU

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Mol	Chain	Res	Type
1	A	232	ARG
1	A	241	ARG
1	B	32	ASN
1	B	39	ARG
1	B	48	THR
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	100	SER
1	B	108	LEU
1	B	113	LEU
1	B	139	LEU
1	B	146	ARG
1	B	163	HIS
1	B	165	LEU
1	B	175	LEU
1	B	192	ARG
1	B	221	LEU
1	B	223	ARG
1	B	232	ARG
1	B	241	ARG
1	B	256	ILE
1	C	36	SER
1	C	50	LYS
1	C	74	GLN
1	C	78	LEU
1	C	82	SER
1	C	98	GLU
1	C	99	LEU
1	C	139	LEU
1	C	150	ASP
1	C	160	ARG
1	C	164	SER
1	C	166	LEU
1	C	191	ARG
1	C	196	LEU
1	C	203	CYS
1	C	205	LYS
1	C	220	CYS

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Mol	Chain	Res	Type
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	D	34	LEU
1	D	50	LYS
1	D	59	LEU
1	D	64	PHE
1	D	66	LYS
1	D	67	GLU
1	D	68	ASP
1	D	99	LEU
1	D	106	LEU
1	D	108	LEU
1	D	113	LEU
1	D	131	LEU
1	D	139	LEU
1	D	164	SER
1	D	175	LEU
1	D	176	SER
1	D	182	THR
1	D	183	ASP
1	D	191	ARG
1	D	224	LEU
1	D	234	LEU
1	D	256	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	63	HIS
1	A	140	HIS
1	B	104	GLN
1	B	140	HIS
1	C	57	GLN
1	C	63	HIS
1	C	74	GLN
1	C	140	HIS

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Mol	Chain	Res	Type
1	C	188	GLN
1	C	240	GLN
1	D	140	HIS
1	D	163	HIS
1	D	188	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.13	5 (2%) 59 60	30, 52, 72, 77	0
1	B	230/273 (84%)	0.15	5 (2%) 59 60	31, 51, 65, 74	0
1	C	227/273 (83%)	0.21	5 (2%) 59 60	38, 54, 72, 81	0
1	D	227/273 (83%)	0.28	12 (5%) 25 26	46, 62, 81, 85	0
All	All	914/1092 (83%)	0.20	27 (2%) 48 49	30, 54, 77, 85	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	PRO	5.6
1	A	48	THR	5.3
1	D	63	HIS	4.6
1	D	64	PHE	4.5
1	B	63	HIS	4.4
1	B	64	PHE	3.6
1	B	217	PRO	3.6
1	D	211	VAL	3.5
1	D	199	ARG	3.2
1	B	61	LEU	3.0
1	D	221	LEU	2.9
1	C	50	LYS	2.9
1	C	65	GLY	2.8
1	A	100	SER	2.7
1	D	93	ILE	2.6
1	C	51	LEU	2.6
1	D	187	LEU	2.4
1	C	134	CYS	2.4
1	A	260	ILE	2.4
1	C	64	PHE	2.4
1	D	181	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	217	PRO	2.2
1	A	61	LEU	2.2
1	D	61	LEU	2.1
1	D	198	ASN	2.1
1	D	257	ILE	2.0
1	D	210	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.