Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:25 PM EDT

PDB ID	:	3MSV
Title	:	The hypoxic regulator of sterol synthesis Nro1 is a nuclear import adaptor
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Deposited on	:	2010-04-29
Resolution	:	2.18 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:

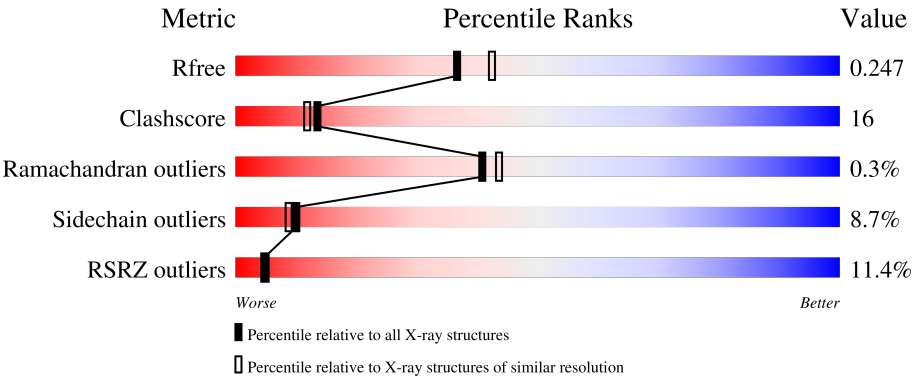
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 <=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	393	11% 65% 21% • 10%
1	B	393	10% 64% 21% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6039 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 Nuclear import adaptor, Nro1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	1	0
			2834	1799	457	573	5			
1	B	348	Total	C	N	O	S	0	1	0
			2810	1789	449	567	5			

- Molecule 2 is water.

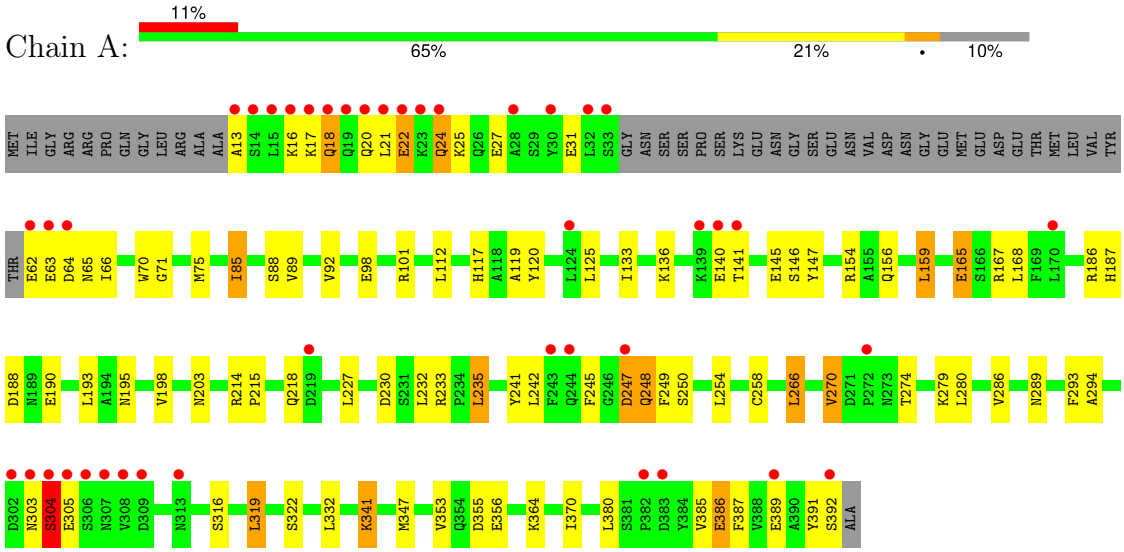
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	199	Total	O	0	0
			199	199		
2	B	196	Total	O	0	0
			196	196		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

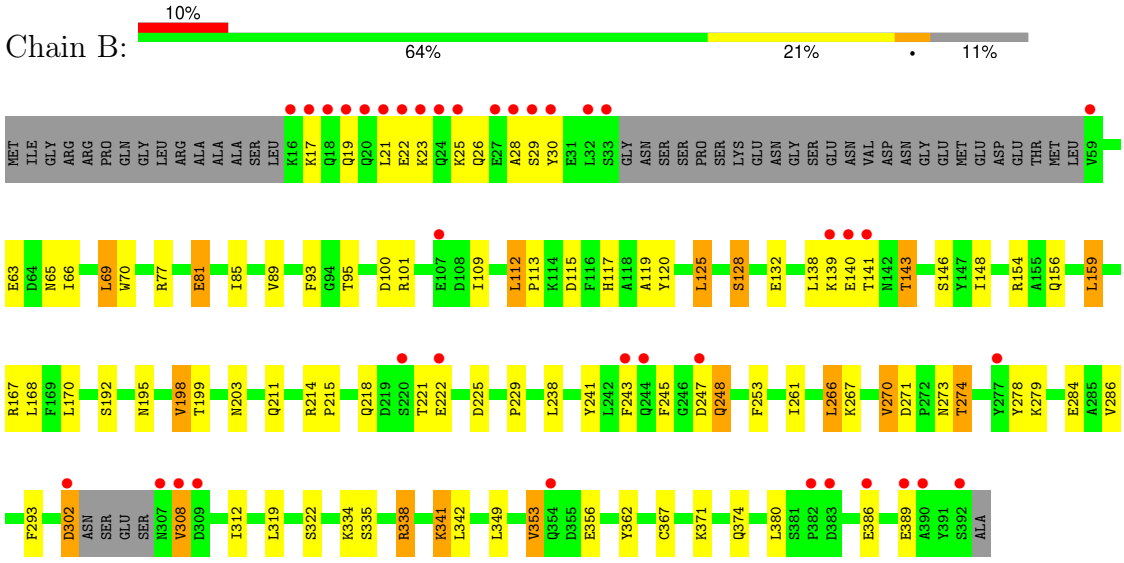
• Molecule 1: Nuclear import adaptor, Nro1

Chain A:



• Molecule 1: Nuclear import adaptor, Nro1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.79Å 107.96Å 100.78Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	19.73 – 2.18 19.69 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.73-2.18) 98.6 (19.69-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.205 , 0.257 0.200 , 0.247	Depositor DCC
R_{free} test set	2576 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6039	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/2889	0.62	0/3926
1	B	0.50	0/2865	0.63	1/3893 (0.0%)
All	All	0.50	0/5754	0.62	1/7819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2834	0	2761	89	0
1	B	2810	0	2735	92	0
2	A	199	0	0	25	0
2	B	196	0	0	20	0
All	All	6039	0	5496	178	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 16.

All (178) 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:367:CYS:SG	2:B:589:HOH:O	1.96	1.22
1:A:233[B]:ARG:HG3	2:A:425:HOH:O	1.48	1.11
1:B:167:ARG:HH22	1:B:225:ASP:HB2	1.21	1.04
1:B:143:THR:HG22	1:B:146:SER:HB2	1.40	0.99
1:A:165:GLU:CG	2:A:527:HOH:O	2.08	0.99
1:A:364:LYS:HE2	2:A:551:HOH:O	1.60	0.97
1:A:233[A]:ARG:HD2	2:A:467:HOH:O	1.63	0.97
1:B:143:THR:HG23	1:B:146:SER:H	1.29	0.97
1:A:165:GLU:CD	2:A:527:HOH:O	2.02	0.96
1:A:233[B]:ARG:CG	2:A:425:HOH:O	2.07	0.92
1:B:167:ARG:NH2	1:B:225:ASP:HB2	1.86	0.89
1:B:141:THR:HG23	1:B:141:THR:O	1.71	0.89
1:B:115:ASP:OD1	2:B:408:HOH:O	1.94	0.86
1:B:143:THR:CG2	1:B:146:SER:H	1.91	0.84
1:B:143:THR:HG22	1:B:146:SER:CB	2.08	0.84
1:B:386:GLU:HG3	2:B:494:HOH:O	1.76	0.83
1:B:101:ARG:HD2	2:B:519:HOH:O	1.77	0.83
1:B:77:ARG:HD2	2:B:502:HOH:O	1.78	0.81
1:B:243:PHE:CD1	2:B:471:HOH:O	2.33	0.81
1:A:85:ILE:HD11	1:A:133:ILE:HG13	1.61	0.80
1:B:284:GLU:OE2	1:B:338:ARG:NH2	2.14	0.80
1:A:248:GLN:HG3	2:A:431:HOH:O	1.82	0.79
1:B:271:ASP:O	1:B:274:THR:CG2	2.32	0.77
1:B:22:GLU:OE2	1:B:25:LYS:NZ	2.16	0.77
1:B:308:VAL:HG13	1:B:312:ILE:HD12	1.67	0.75
1:B:243:PHE:HD1	2:B:471:HOH:O	1.68	0.74
1:A:85:ILE:HD11	1:A:133:ILE:CG1	2.19	0.73
1:A:165:GLU:HG2	2:A:527:HOH:O	1.84	0.70
1:A:18:GLN:HE21	1:A:18:GLN:HA	1.57	0.69
1:A:245:PHE:O	1:A:248:GLN:HG2	1.92	0.69
1:B:143:THR:HG23	1:B:146:SER:N	2.03	0.69
1:B:248:GLN:HE21	1:B:248:GLN:N	1.90	0.69
1:A:355:ASP:OD1	2:A:418:HOH:O	2.10	0.69
1:B:117:HIS:HD2	1:B:154:ARG:HH11	1.40	0.68
1:A:17:LYS:O	1:A:21:LEU:HB2	1.93	0.68
1:A:22:GLU:HA	1:A:22:GLU:OE1	1.92	0.67
1:B:353:VAL:HG11	1:B:362:TYR:HE1	1.58	0.67
1:B:271:ASP:O	1:B:274:THR:HG22	1.94	0.67
1:B:271:ASP:O	1:B:274:THR:HG23	1.95	0.67
1:B:101:ARG:NH1	2:B:498:HOH:O	2.27	0.66
1:B:117:HIS:HE1	2:B:399:HOH:O	1.80	0.65
1:B:198:VAL:HG11	1:B:245:PHE:CZ	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:HB3	1:B:215:PRO:HD3	1.79	0.65
1:B:69:LEU:HD22	1:B:95:THR:HG23	1.78	0.65
1:B:167:ARG:NH2	1:B:225:ASP:CB	2.58	0.64
1:A:218:GLN:NE2	2:A:543:HOH:O	2.23	0.64
1:A:85:ILE:CD1	1:A:133:ILE:HG13	2.28	0.64
1:B:143:THR:CG2	1:B:146:SER:N	2.60	0.63
1:A:203:ASN:ND2	1:A:241:TYR:OH	2.32	0.63
1:B:247:ASP:OD1	1:B:248:GLN:NE2	2.32	0.62
1:A:85:ILE:HD11	1:A:133:ILE:CB	2.29	0.62
1:B:143:THR:CG2	1:B:146:SER:HB2	2.25	0.62
1:B:334:LYS:HE2	2:B:488:HOH:O	1.99	0.62
1:B:141:THR:O	1:B:141:THR:CG2	2.44	0.62
1:B:386:GLU:CG	2:B:494:HOH:O	2.37	0.62
1:A:294:ALA:CB	1:A:319:LEU:HD13	2.30	0.62
1:A:156:GLN:HA	1:A:159:LEU:HD22	1.81	0.61
1:B:19:GLN:O	1:B:23:LYS:HG2	1.99	0.61
1:A:27:GLU:O	1:A:31:GLU:HB2	2.00	0.61
1:B:125:LEU:O	1:B:128:SER:HB2	2.00	0.61
1:B:17:LYS:HG2	1:B:17:LYS:O	2.00	0.61
1:A:117:HIS:HD2	1:A:154:ARG:HH11	1.47	0.61
1:A:270:VAL:CG1	2:A:504:HOH:O	2.49	0.61
1:B:266:LEU:HD13	1:B:286:VAL:HG21	1.83	0.60
1:A:85:ILE:HD11	1:A:133:ILE:HB	1.83	0.60
1:B:270:VAL:O	1:B:271:ASP:C	2.39	0.60
1:B:319:LEU:O	1:B:322:SER:HB2	2.01	0.60
1:B:218:GLN:O	1:B:267:LYS:NZ	2.35	0.59
1:B:221:THR:O	1:B:267:LYS:HE2	2.03	0.58
1:B:353:VAL:CG1	1:B:362:TYR:HE1	2.16	0.58
1:B:146:SER:HB3	2:B:465:HOH:O	2.03	0.58
1:B:203:ASN:ND2	1:B:241:TYR:OH	2.37	0.57
1:A:21:LEU:CD2	1:A:25:LYS:HE3	2.34	0.57
1:A:380:LEU:HB3	1:A:385:VAL:HG23	1.86	0.57
1:A:289:ASN:ND2	2:A:510:HOH:O	2.38	0.57
1:A:195:ASN:ND2	1:B:100:ASP:OD1	2.34	0.56
1:A:233[A]:ARG:CD	2:A:467:HOH:O	2.36	0.56
1:B:81:GLU:OE1	1:B:278:TYR:OH	2.16	0.56
1:A:347:MET:HE3	1:A:370:ILE:HD11	1.87	0.56
1:A:117:HIS:CD2	1:A:154:ARG:HH11	2.23	0.55
1:A:20:GLN:O	1:A:24:GLN:HG2	2.06	0.55
1:B:93:PHE:HZ	1:B:138:LEU:HD21	1.71	0.55
1:A:117:HIS:HE1	2:A:403:HOH:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:OD1	1:A:247:ASP:N	2.31	0.54
1:A:294:ALA:HB1	1:A:319:LEU:HD13	1.90	0.54
1:B:28:ALA:HA	1:B:253:PHE:CD1	2.41	0.54
1:A:232:LEU:O	1:A:235:LEU:HB2	2.07	0.54
1:B:132[B]:GLU:HG3	2:B:412:HOH:O	2.07	0.54
1:A:316:SER:HB2	2:A:588:HOH:O	2.07	0.53
1:A:341:LYS:HE2	2:A:400:HOH:O	2.08	0.52
1:B:117:HIS:CD2	1:B:154:ARG:HH11	2.24	0.52
1:B:335:SER:O	1:B:338:ARG:HG3	2.10	0.52
1:A:31:GLU:CG	1:A:249:PHE:HD1	2.23	0.52
1:A:230:ASP:HA	1:A:233[B]:ARG:HE	1.74	0.51
1:A:266:LEU:HD13	1:A:286:VAL:HG21	1.92	0.51
1:B:338:ARG:HB3	2:B:507:HOH:O	2.09	0.51
1:B:271:ASP:OD1	1:B:273:ASN:HB2	2.10	0.51
1:A:167:ARG:NE	2:A:458:HOH:O	2.43	0.51
1:A:31:GLU:OE2	1:A:250:SER:N	2.41	0.50
1:B:243:PHE:CE1	2:B:471:HOH:O	2.60	0.50
1:A:71:GLY:O	1:A:75:MET:HG3	2.12	0.50
1:B:248:GLN:HE21	1:B:248:GLN:H	1.57	0.50
1:B:374:GLN:HB2	1:B:380:LEU:HD11	1.93	0.50
1:B:77:ARG:CD	2:B:502:HOH:O	2.50	0.50
1:A:62:GLU:C	1:A:64:ASP:H	2.16	0.49
1:A:165:GLU:CB	2:A:527:HOH:O	2.51	0.49
1:A:140:GLU:N	1:A:140:GLU:OE1	2.46	0.49
1:A:303:ASN:O	1:A:304:SER:O	2.31	0.48
1:B:21:LEU:HD23	1:B:21:LEU:O	2.14	0.48
1:B:128:SER:OG	1:B:148:ILE:HG13	2.14	0.48
1:A:18:GLN:O	1:A:22:GLU:HB2	2.14	0.48
1:B:21:LEU:HD23	1:B:21:LEU:C	2.33	0.48
1:B:349:LEU:O	1:B:353:VAL:HG22	2.14	0.48
1:A:13:ALA:N	1:A:16:LYS:HB2	2.28	0.48
2:A:517:HOH:O	1:B:143:THR:HG21	2.13	0.47
1:B:22:GLU:OE2	1:B:25:LYS:CE	2.61	0.47
1:B:63:GLU:HB2	2:B:493:HOH:O	2.13	0.47
1:A:364:LYS:CE	2:A:551:HOH:O	2.35	0.47
1:B:109:ILE:HA	1:B:112:LEU:HD22	1.97	0.47
1:A:146:SER:HB3	2:B:562:HOH:O	2.12	0.47
1:B:211:GLN:HB2	2:B:585:HOH:O	2.13	0.47
1:B:341:LYS:HD2	1:B:341:LYS:O	2.14	0.47
1:A:85:ILE:CG1	1:A:133:ILE:HG13	2.45	0.47
1:A:386:GLU:HG3	1:A:387:PHE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD23	1:A:21:LEU:O	2.14	0.46
1:A:341:LYS:O	1:A:341:LYS:CD	2.63	0.46
1:B:353:VAL:HG11	1:B:362:TYR:CE1	2.45	0.46
1:A:22:GLU:OE1	1:A:25:LYS:HD2	2.16	0.46
1:B:274:THR:O	1:B:279:LYS:HE3	2.16	0.46
1:B:302:ASP:OD1	1:B:302:ASP:N	2.48	0.46
1:B:199:THR:HG22	1:B:241:TYR:OH	2.16	0.45
1:A:65:ASN:OD1	1:A:66:ILE:N	2.50	0.45
1:B:26:GLN:O	1:B:29:SER:HB3	2.16	0.45
1:B:199:THR:HG22	1:B:241:TYR:HH	1.82	0.45
1:B:271:ASP:HB3	1:B:274:THR:HG22	1.99	0.45
1:A:187:HIS:HE1	2:A:575:HOH:O	1.98	0.45
1:A:187:HIS:HD2	1:A:188:ASP:OD1	2.00	0.45
1:B:66:ILE:CD1	1:B:113:PRO:HD2	2.47	0.45
1:B:28:ALA:HB1	1:B:253:PHE:HE1	1.82	0.45
1:A:31:GLU:HG2	1:A:249:PHE:HD1	1.82	0.44
1:A:190:GLU:OE2	1:B:146:SER:OG	2.27	0.44
1:B:85:ILE:O	1:B:89:VAL:HG23	2.17	0.44
1:A:389:GLU:HB2	2:A:585:HOH:O	2.18	0.44
1:B:238:LEU:HG	1:B:261:ILE:HD11	2.00	0.44
1:B:267:LYS:HA	1:B:270:VAL:HG22	1.99	0.44
1:A:332:LEU:HD23	2:A:554:HOH:O	2.17	0.43
1:A:391:TYR:CD2	1:A:392:SER:HB2	2.53	0.43
1:A:141:THR:O	1:A:141:THR:OG1	2.28	0.43
1:B:156:GLN:O	1:B:159:LEU:HB2	2.18	0.43
1:B:308:VAL:HG13	1:B:312:ILE:CD1	2.43	0.43
1:B:28:ALA:HA	1:B:253:PHE:HD1	1.82	0.43
1:A:88:SER:O	1:A:92:VAL:HG23	2.18	0.43
1:A:230:ASP:HA	1:A:233[B]:ARG:NE	2.33	0.43
1:A:341:LYS:HA	1:A:341:LYS:HD3	1.78	0.43
1:A:62:GLU:O	1:A:63:GLU:HB3	2.19	0.43
1:A:303:ASN:O	1:A:304:SER:C	2.57	0.43
1:A:305:GLU:O	1:A:305:GLU:HG2	2.18	0.43
1:B:229:PRO:HG2	1:B:278:TYR:HB3	2.01	0.42
1:A:145:GLU:OE1	1:A:186:ARG:HD2	2.19	0.42
1:A:254:LEU:O	1:A:258:CYS:SG	2.77	0.42
1:A:341:LYS:CD	1:A:341:LYS:C	2.86	0.42
1:A:214:ARG:HB3	1:A:215:PRO:CD	2.50	0.42
1:A:233[B]:ARG:CZ	2:A:425:HOH:O	2.68	0.42
1:A:98:GLU:OE2	1:A:101:ARG:NH1	2.53	0.42
1:B:139:LYS:O	2:B:590:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:O	1:A:322:SER:HB2	2.20	0.42
1:B:221:THR:O	1:B:267:LYS:CE	2.68	0.41
1:A:70:TRP:NE1	1:A:119:ALA:HB2	2.35	0.41
1:A:85:ILE:HD12	1:A:89:VAL:HG23	2.02	0.41
1:A:147:TYR:CE1	1:B:192:SER:HB3	2.56	0.41
1:A:187:HIS:CD2	1:A:198:VAL:HG22	2.55	0.41
1:A:31:GLU:HG3	1:A:249:PHE:HD1	1.85	0.41
1:B:81:GLU:O	1:B:81:GLU:HG3	2.20	0.41
1:A:341:LYS:O	1:A:341:LYS:HD3	2.21	0.41
1:A:341:LYS:O	1:A:341:LYS:HD2	2.20	0.40
1:B:70:TRP:CE2	1:B:119:ALA:HB2	2.56	0.40
1:A:274:THR:O	1:A:279:LYS:HE3	2.22	0.40
1:A:353:VAL:HG23	2:A:553:HOH:O	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	349/393 (89%)	341 (98%)	7 (2%)	1 (0%)	41	43
1	B	343/393 (87%)	333 (97%)	9 (3%)	1 (0%)	41	43
All	All	692/786 (88%)	674 (97%)	16 (2%)	2 (0%)	41	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	SER
1	B	308	VAL

5.3.2 Protein sidechains (i)

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	312/344 (91%)	286 (92%)	26 (8%)	11 10
1	B	309/344 (90%)	281 (91%)	28 (9%)	9 8
All	All	621/688 (90%)	567 (91%)	54 (9%)	10 9

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	22	GLU
1	A	24	GLN
1	A	85	ILE
1	A	112	LEU
1	A	120	TYR
1	A	125	LEU
1	A	136	LYS
1	A	159	LEU
1	A	165	GLU
1	A	168	LEU
1	A	193	LEU
1	A	227	LEU
1	A	235	LEU
1	A	242	LEU
1	A	247	ASP
1	A	248	GLN
1	A	266	LEU
1	A	270	VAL
1	A	280	LEU
1	A	293	PHE
1	A	304	SER
1	A	319	LEU
1	A	341	LYS
1	A	356	GLU
1	A	386	GLU
1	B	30	TYR

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Mol	Chain	Res	Type
1	B	65	ASN
1	B	69	LEU
1	B	81	GLU
1	B	112	LEU
1	B	120	TYR
1	B	125	LEU
1	B	128	SER
1	B	140	GLU
1	B	143	THR
1	B	159	LEU
1	B	168	LEU
1	B	170	LEU
1	B	195	ASN
1	B	198	VAL
1	B	222	GLU
1	B	248	GLN
1	B	266	LEU
1	B	270	VAL
1	B	274	THR
1	B	293	PHE
1	B	302	ASP
1	B	341	LYS
1	B	342	LEU
1	B	353	VAL
1	B	356	GLU
1	B	371	LYS
1	B	389	GLU

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	18	GLN
1	A	24	GLN
1	A	117	HIS
1	A	156	GLN
1	A	187	HIS
1	A	203	ASN
1	A	244	GLN
1	A	303	ASN
1	A	321	ASN
1	B	117	HIS
1	B	135	GLN

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Mol	Chain	Res	Type
1	B	195	ASN
1	B	200	GLN
1	B	203	ASN
1	B	248	GLN
1	B	321	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	352/393 (89%)	0.58	42 (11%)	4	4	16, 29, 60, 77	13 (3%)
1	B	348/393 (88%)	0.51	38 (10%)	5	6	15, 29, 55, 88	6 (1%)
All	All	700/786 (89%)	0.54	80 (11%)	5	5	15, 29, 58, 88	19 (2%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	7.6
1	B	392	SER	7.5
1	B	32	LEU	7.3
1	B	21	LEU	7.1
1	A	306	SER	7.0
1	B	308	VAL	5.9
1	A	15	LEU	5.6
1	A	307	ASN	5.6
1	A	30	TYR	5.3
1	A	16	LYS	5.3
1	B	19	GLN	5.2
1	B	18	GLN	5.1
1	A	308	VAL	4.9
1	A	305	GLU	4.9
1	B	33	SER	4.6
1	A	21	LEU	4.6
1	A	19	GLN	4.5
1	A	243	PHE	4.5
1	A	18	GLN	4.4
1	A	392	SER	4.3
1	B	30	TYR	4.3
1	B	27	GLU	4.3
1	B	309	ASP	4.2
1	A	13	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	LYS	3.9
1	B	29	SER	3.8
1	B	140	GLU	3.8
1	B	17	LYS	3.8
1	A	20	GLN	3.8
1	A	304	SER	3.7
1	A	302	ASP	3.7
1	B	141	THR	3.7
1	A	22	GLU	3.5
1	B	59	VAL	3.5
1	A	23	LYS	3.4
1	B	20	GLN	3.4
1	A	247	ASP	3.3
1	A	63	GLU	3.3
1	B	107	GLU	3.3
1	B	382	PRO	3.2
1	A	140	GLU	3.2
1	A	28	ALA	3.2
1	A	303	ASN	3.1
1	B	22	GLU	3.0
1	B	243	PHE	3.0
1	A	64	ASP	2.9
1	B	307	ASN	2.9
1	B	244	GLN	2.8
1	B	302	ASP	2.8
1	B	383	ASP	2.7
1	A	383	ASP	2.7
1	A	24	GLN	2.7
1	A	389	GLU	2.7
1	B	390	ALA	2.7
1	A	272	PRO	2.6
1	B	28	ALA	2.6
1	B	23	LYS	2.5
1	B	389	GLU	2.5
1	B	247	ASP	2.4
1	B	24	GLN	2.4
1	B	25	LYS	2.4
1	B	139	LYS	2.4
1	A	62	GLU	2.4
1	A	17	LYS	2.4
1	B	277	TYR	2.4
1	A	141	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	33	SER	2.3
1	A	309	ASP	2.2
1	B	386	GLU	2.2
1	A	244	GLN	2.2
1	B	220	SER	2.2
1	A	219	ASP	2.1
1	A	170	LEU	2.1
1	A	14	SER	2.1
1	B	222	GLU	2.1
1	A	313	ASN	2.0
1	A	124	LEU	2.0
1	B	354	GLN	2.0
1	A	382	PRO	2.0
1	A	139	LYS	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 monosaccharides 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.