Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2023 – 07:13 pm BST

PDB ID	:	8OW4
Title	:	2.75 angstrom crystal structure of human NFAT1 with bound DNA
Authors	:	Lopez-Sagaseta, J.; Erausquin, E.; Hernandez-Morales, S.; Urdiciain, A.; Lasarte, J.J.; Lozano, T.
Deposited on	:	2023-04-27
Resolution	:	2.75 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:

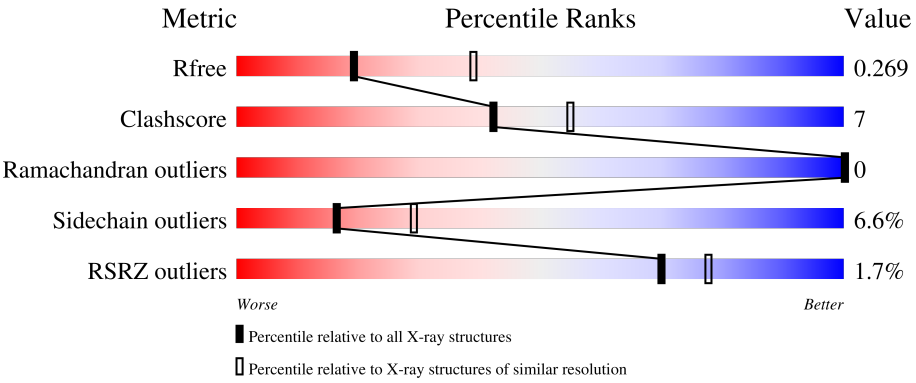
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	298	2% 61% 13% 24%
1	B	298	% 78% 19%
2	G	15	33% 53% 13%
2	W	15	33% 40% 27%
3	C	15	47% 40% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	15	33% 33% 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5254 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 factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1708	1079	307	316	6			
1	B	296	Total	C	N	O	S	0	0	0
			2319	1454	429	427	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	MET	-	initiating methionine	UNP Q13469
A	382	ALA	-	expression tag	UNP Q13469
A	383	HIS	-	expression tag	UNP Q13469
A	384	HIS	-	expression tag	UNP Q13469
A	385	HIS	-	expression tag	UNP Q13469
A	386	HIS	-	expression tag	UNP Q13469
A	387	HIS	-	expression tag	UNP Q13469
A	388	HIS	-	expression tag	UNP Q13469
A	389	VAL	-	expression tag	UNP Q13469
A	390	GLY	-	expression tag	UNP Q13469
B	381	MET	-	initiating methionine	UNP Q13469
B	382	ALA	-	expression tag	UNP Q13469
B	383	HIS	-	expression tag	UNP Q13469
B	384	HIS	-	expression tag	UNP Q13469
B	385	HIS	-	expression tag	UNP Q13469
B	386	HIS	-	expression tag	UNP Q13469
B	387	HIS	-	expression tag	UNP Q13469
B	388	HIS	-	expression tag	UNP Q13469
B	389	VAL	-	expression tag	UNP Q13469
B	390	GLY	-	expression tag	UNP Q13469

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*AP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			
2	G	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			
3	H	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			

- Molecule 4 is water.

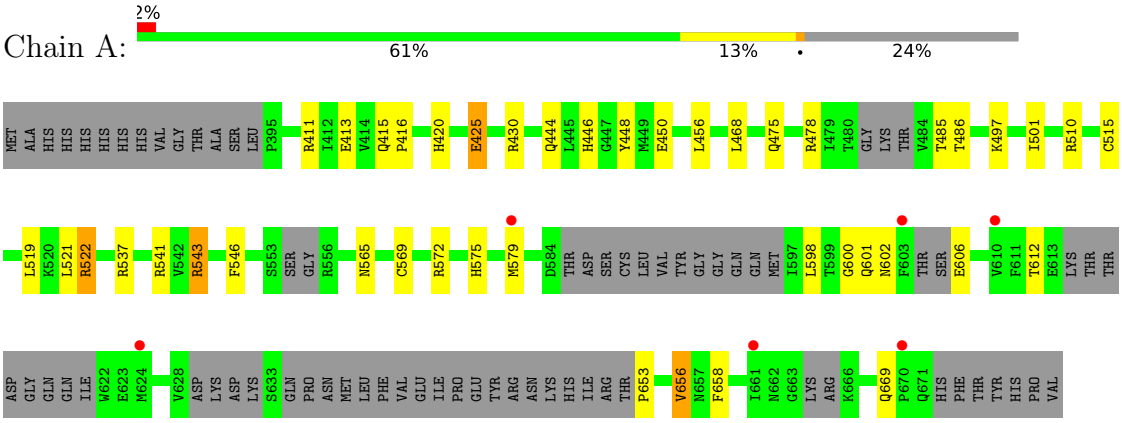
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	6	Total	O	0	0
			6	6		

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.

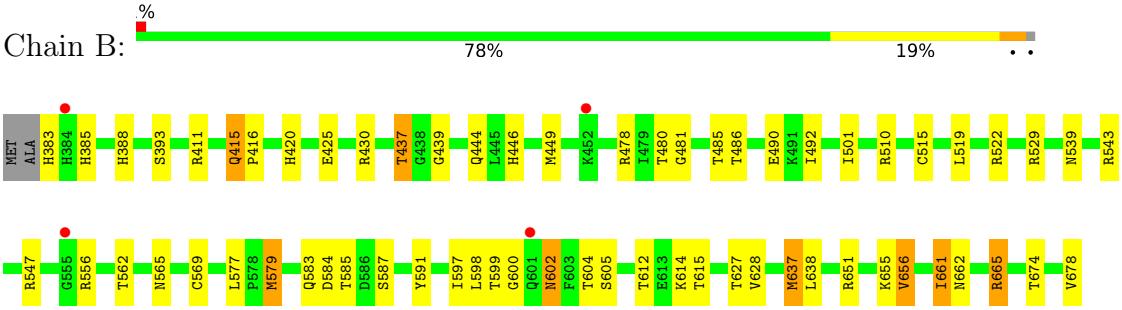
• Molecule 1: Nuclear factor of activated T-cells, cytoplasmic 2

Chain A:



• Molecule 1: Nuclear factor of activated T-cells, cytoplasmic 2

Chain B:

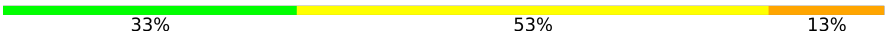


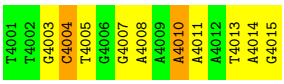
• Molecule 2: DNA (5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*AP*TP*AP*G)-3')

Chain W:

• Molecule 2: DNA (5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*AP*TP*AP*G)-3')

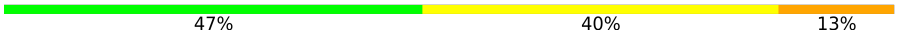
Chain G:





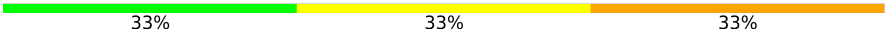
• Molecule 3: DNA (5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3')

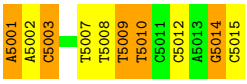
Chain C:



• Molecule 3: DNA (5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3')

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.50Å 94.43Å 129.45Å 90.00° 93.57° 90.00°	Depositor
Resolution (Å)	82.24 – 2.75 82.24 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.2 (82.24-2.75) 97.2 (82.24-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.216 , 0.273 0.218 , 0.269	Depositor DCC
R_{free} test set	1717 reflections (5.54%)	wwPDB-VP
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5254	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.32% 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	0.49	1/1739 (0.1%)	0.78	1/2355 (0.0%)
1	B	0.46	0/2375	0.84	3/3227 (0.1%)
2	G	0.91	0/349	1.58	9/538 (1.7%)
2	W	0.86	0/349	1.62	6/538 (1.1%)
3	C	0.87	0/333	1.49	4/511 (0.8%)
3	H	0.98	0/333	1.70	7/511 (1.4%)
All	All	0.61	1/5478 (0.0%)	1.09	30/7680 (0.4%)

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	5
1	B	0	9
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	GLU	CD-OE2	6.59	1.32	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	4008	DA	O4'-C1'-N9	8.59	114.01	108.00
3	H	5009	DT	O5'-P-OP1	-7.93	98.56	105.70
3	H	5014	DG	P-O3'-C3'	-7.60	110.58	119.70
2	G	4008	DA	O4'-C1'-N9	7.48	113.24	108.00
2	W	4002	DT	P-O3'-C3'	-7.28	110.96	119.70
2	G	4004	DC	O4'-C1'-C2'	-7.03	100.27	105.90
2	G	4007	DG	P-O3'-C3'	6.85	127.92	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5009	DT	O5'-P-OP1	-6.83	99.55	105.70
2	G	4003	DG	OP1-P-OP2	6.69	129.64	119.60
3	C	5014	DG	P-O3'-C3'	-6.46	111.95	119.70
3	H	5003	DC	P-O3'-C3'	-6.34	112.10	119.70
1	A	411	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	H	5009	DT	O4'-C1'-N1	-6.09	103.74	108.00
2	W	4007	DG	P-O3'-C3'	6.04	126.95	119.70
2	G	4015	DG	O4'-C1'-N9	5.97	112.18	108.00
3	H	5010	DT	OP1-P-OP2	-5.84	110.84	119.60
2	G	4010	DA	P-O3'-C3'	-5.64	112.93	119.70
1	B	556	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	G	4004	DC	C1'-O4'-C4'	-5.45	104.65	110.10
2	G	4013	DT	O4'-C1'-C2'	-5.39	101.59	105.90
2	W	4005	DT	O5'-P-OP1	-5.38	100.86	105.70
1	B	655	LYS	CB-CA-C	5.31	121.02	110.40
2	G	4007	DG	O4'-C4'-C3'	5.14	109.09	106.00
3	C	5002	DA	P-O3'-C3'	-5.13	113.54	119.70
3	C	5007	DT	OP1-P-OP2	5.13	127.29	119.60
3	H	5009	DT	OP1-P-OP2	5.08	127.21	119.60
2	W	4010	DA	P-O3'-C3'	-5.05	113.64	119.70
3	H	5001	DA	C2-N3-C4	-5.03	108.09	110.60
2	W	4014	DA	O5'-P-OP2	5.03	116.73	110.70
1	B	547	ARG	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	430	ARG	Sidechain
1	A	478	ARG	Sidechain
1	A	522	ARG	Sidechain
1	A	541	ARG	Sidechain
1	A	543	ARG	Sidechain
1	B	411	ARG	Sidechain
1	B	430	ARG	Sidechain
1	B	478	ARG	Sidechain
1	B	481	GLY	Peptide
1	B	522	ARG	Sidechain
1	B	529	ARG	Sidechain
1	B	543	ARG	Sidechain
1	B	651	ARG	Sidechain
1	B	665	ARG	Sidechain

5.2 Too-close contacts (i)

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	1708	0	1636	25	0
1	B	2319	0	2258	26	0
2	G	310	0	171	3	0
2	W	310	0	171	6	0
3	C	299	0	173	5	0
3	H	299	0	173	9	0
4	A	3	0	0	0	0
4	B	6	0	0	1	0
All	All	5254	0	4582	68	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 (68) 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:577:LEU:O	1:B:602:ASN:ND2	1.98	0.96
3:H:5001:DA:HO5'	3:H:5001:DA:H8	0.96	0.93
2:W:4002:DT:H2"	2:W:4003:DG:OP2	1.69	0.92
3:C:5001:DA:HO5'	3:C:5001:DA:H8	0.99	0.91
2:G:4004:DC:H2"	2:G:4005:DT:H5"	1.62	0.80
1:B:415:GLN:HE21	1:B:416:PRO:HD2	1.47	0.78
2:W:4004:DC:H2"	2:W:4005:DT:H5"	1.69	0.74
1:A:444:GLN:OE1	1:A:446:HIS:CE1	2.41	0.73
1:B:490:GLU:OE2	4:B:701:HOH:O	2.09	0.71
1:A:572:ARG:NH2	3:H:5007:DT:OP2	2.24	0.69
3:C:5015:DC:OP1	3:C:5015:DC:H4'	1.93	0.68
1:B:415:GLN:HE22	1:B:565:ASN:H	1.42	0.67
1:A:415:GLN:HE22	1:A:565:ASN:H	1.42	0.67
3:H:5015:DC:H4'	3:H:5015:DC:OP1	1.95	0.67
1:A:415:GLN:HE21	1:A:416:PRO:HD2	1.61	0.66
2:W:4002:DT:C2'	2:W:4003:DG:OP2	2.39	0.66
1:B:665:ARG:HH11	1:B:665:ARG:HG3	1.59	0.66
1:A:468:LEU:HD13	1:A:543:ARG:HH11	1.64	0.62
1:B:415:GLN:NE2	1:B:416:PRO:HD2	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:HG2	1:A:510:ARG:HH22	1.64	0.62
1:B:591:TYR:CE2	1:B:678:VAL:HG21	2.34	0.62
1:A:413:GLU:HG2	1:A:510:ARG:NH2	2.17	0.60
3:C:5001:DA:H2"	3:C:5002:DA:O5'	2.06	0.56
1:A:415:GLN:NE2	1:A:416:PRO:HD2	2.19	0.56
3:H:5001:DA:H2"	3:H:5002:DA:O5'	2.06	0.56
3:C:5008:DT:H2"	3:C:5009:DT:H5'	1.88	0.55
1:B:612:THR:O	1:B:656:VAL:HG22	2.08	0.54
3:H:5012:DC:OP2	1:B:385:HIS:NE2	2.36	0.53
1:B:444:GLN:OE1	1:B:446:HIS:NE2	2.42	0.53
1:A:612:THR:O	1:A:656:VAL:HG22	2.08	0.53
3:H:5008:DT:H2"	3:H:5009:DT:H5'	1.89	0.53
1:A:456:LEU:HD11	1:A:546:PHE:HB3	1.89	0.53
1:B:501:ILE:HD11	1:B:515:CYS:SG	2.49	0.52
1:A:448:TYR:CZ	1:A:450:GLU:HB2	2.45	0.52
1:A:598:LEU:HD21	1:A:658:PHE:HE2	1.77	0.50
1:A:579:MET:O	1:A:600:GLY:HA3	2.11	0.49
1:A:420:HIS:O	1:A:569:CYS:HA	2.12	0.49
1:B:604:THR:HG22	1:B:605:SER:H	1.77	0.48
2:W:4014:DA:C2	3:C:5005:DA:C2	3.02	0.48
1:B:579:MET:O	1:B:600:GLY:HA3	2.13	0.47
2:G:4010:DA:H2"	2:G:4011:DA:O5'	2.14	0.47
1:B:599:THR:HG22	1:B:637:MET:HG3	1.96	0.47
1:A:501:ILE:HD11	1:A:515:CYS:SG	2.55	0.47
1:B:437:THR:HB	1:B:439:GLY:H	1.80	0.46
1:A:522:ARG:NH1	3:H:5010:DT:OP1	2.49	0.46
1:B:420:HIS:O	1:B:569:CYS:HA	2.17	0.45
1:A:415:GLN:NE2	1:A:565:ASN:H	2.12	0.45
1:A:444:GLN:HE21	1:A:510:ARG:HB2	1.81	0.44
1:A:537:ARG:CD	2:G:4014:DA:H5"	2.48	0.44
1:A:475:GLN:HG2	1:A:521:LEU:HD11	1.99	0.44
1:B:604:THR:HG22	1:B:605:SER:N	2.33	0.44
1:A:425:GLU:HG3	1:A:519:LEU:HD11	1.99	0.44
1:A:497:LYS:HE2	1:B:492:ILE:HG21	2.00	0.44
2:W:4010:DA:H2"	2:W:4011:DA:O5'	2.18	0.43
1:B:628:VAL:O	1:B:628:VAL:HG23	2.18	0.43
1:B:584:ASP:CB	1:B:597:ILE:H	2.31	0.43
1:B:661:ILE:C	1:B:662:ASN:HD22	2.20	0.43
1:A:598:LEU:HD21	1:A:658:PHE:CE2	2.53	0.43
1:B:444:GLN:NE2	1:B:510:ARG:HH11	2.17	0.43
1:A:444:GLN:NE2	1:A:510:ARG:HH11	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:SER:HA	1:B:674:THR:O	2.18	0.43
3:H:5002:DA:H2"	3:H:5003:DC:O5'	2.20	0.42
1:B:425:GLU:HG3	1:B:519:LEU:HD11	2.02	0.42
1:B:388:HIS:O	1:B:393:SER:CB	2.68	0.42
2:W:4005:DT:H2'	2:W:4006:DG:C8	2.55	0.41
3:H:5014:DG:H2"	3:H:5015:DC:O5'	2.21	0.40
1:A:575:HIS:O	1:A:602:ASN:ND2	2.55	0.40
1:B:415:GLN:NE2	1:B:565:ASN:H	2.12	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	208/298 (70%)	203 (98%)	5 (2%)	0	100	100
1	B	294/298 (99%)	279 (95%)	15 (5%)	0	100	100
All	All	502/596 (84%)	482 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	177/265 (67%)	170 (96%)	7 (4%)	31	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	250/265 (94%)	229 (92%)	21 (8%)	11 19
All	All	427/530 (81%)	399 (93%)	28 (7%)	16 29

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	THR
1	A	486	THR
1	A	601	GLN
1	A	606	GLU
1	A	653	PRO
1	A	656	VAL
1	A	669	GLN
1	B	383	HIS
1	B	415	GLN
1	B	437	THR
1	B	449	MET
1	B	480	THR
1	B	485	THR
1	B	486	THR
1	B	539	ASN
1	B	562	THR
1	B	579	MET
1	B	583	GLN
1	B	585	THR
1	B	598	LEU
1	B	602	ASN
1	B	614	LYS
1	B	615	THR
1	B	627	THR
1	B	637	MET
1	B	638	LEU
1	B	656	VAL
1	B	661	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	415	GLN
1	A	444	GLN
1	A	446	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	495	ASN
1	A	523	ASN
1	A	583	GLN
1	A	662	ASN
1	A	669	GLN
1	A	671	GLN
1	B	387	HIS
1	B	415	GLN
1	B	444	GLN
1	B	523	ASN
1	B	539	ASN
1	B	583	GLN
1	B	620	GLN
1	B	662	ASN
1	B	669	GLN
1	B	671	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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 (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	225/298 (75%)	0.28	6 (2%) 54 63	61, 95, 147, 179	0
1	B	296/298 (99%)	0.09	4 (1%) 75 82	60, 84, 117, 149	0
2	G	15/15 (100%)	-0.41	0 100 100	71, 82, 91, 92	0
2	W	15/15 (100%)	-0.40	0 100 100	77, 86, 131, 138	0
3	C	15/15 (100%)	-0.43	0 100 100	60, 89, 110, 115	0
3	H	15/15 (100%)	-0.23	0 100 100	60, 77, 96, 107	0
All	All	581/656 (88%)	0.12	10 (1%) 70 78	60, 86, 134, 179	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	PHE	3.6
1	A	661	ILE	3.4
1	A	610	VAL	3.4
1	A	579	MET	3.2
1	B	555	GLY	3.1
1	A	624	MET	3.1
1	B	384	HIS	2.9
1	A	670	PRO	2.6
1	B	601	GLN	2.3
1	B	452	LYS	2.1

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 (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.