Full wwPDB X-ray Structure Validation Report (i)

Sep 4, 2023 – 08:26 PM EDT

PDB ID	:	3TG7
Title	:	Crystal structure of Adenovirus serotype 5 hexon at 1.6A resolution
Authors	:	Zhu, Y.; Roszak, A.W.; Isaacs, N.W.; McVey, J.H.; Nicklin, S.A.; Baker, A.H.
Deposited on	:	2011-08-17
Resolution	:	1.57 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 (i) 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 (1)) were used in the production of this report:

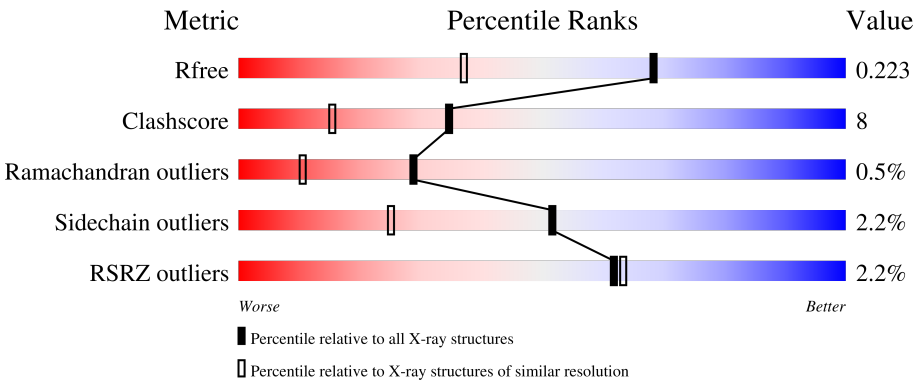
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	951	2% 75% 16% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8005 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 Hexon protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	889	7205	4590	1219	1357	39	0	14	0

- Molecule 2 is water.

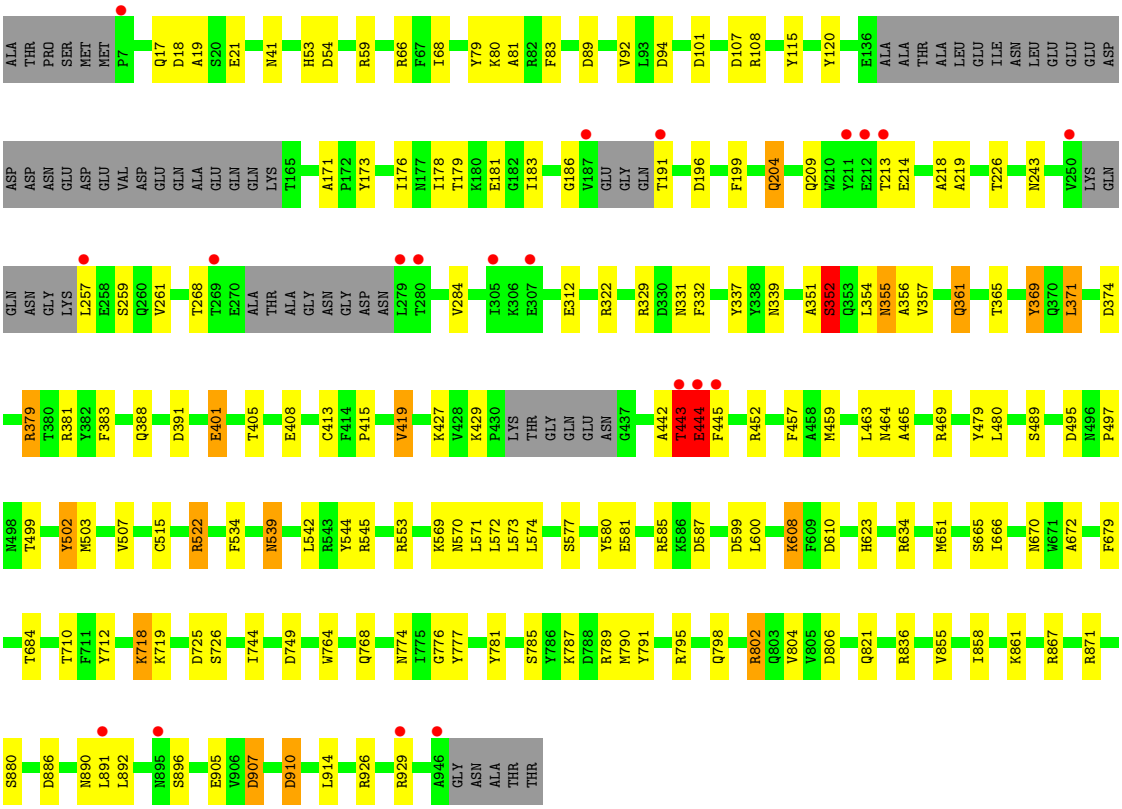
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	800	800	800	0	0

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: Hexon protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	149.15Å 149.15Å 126.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.55 – 1.57 27.95 – 1.57	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.55-1.57) 96.9 (27.95-1.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.184 , 0.223 0.185 , 0.223	Depositor DCC
R_{free} test set	7132 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.093 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8005	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 (i)

5.1 Standard geometry (i)

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	1.34	30/7406 (0.4%)	1.24	42/10072 (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	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLN	CB-CG	-6.93	1.33	1.52
1	A	332	PHE	CD1-CE1	6.56	1.52	1.39
1	A	419	VAL	CB-CG2	-6.11	1.40	1.52
1	A	204	GLN	CD-OE1	6.01	1.37	1.24
1	A	544	TYR	CE1-CZ	-5.90	1.30	1.38
1	A	171	ALA	CA-CB	5.83	1.64	1.52
1	A	369	TYR	CD2-CE2	5.73	1.48	1.39
1	A	502	TYR	CD1-CE1	5.72	1.48	1.39
1	A	92	VAL	CB-CG1	5.63	1.64	1.52
1	A	507	VAL	CB-CG2	5.62	1.64	1.52
1	A	383	PHE	CG-CD1	-5.43	1.30	1.38
1	A	777	TYR	CG-CD1	5.40	1.46	1.39
1	A	768	GLN	N-CA	5.38	1.57	1.46
1	A	383	PHE	CG-CD2	5.34	1.46	1.38
1	A	679	PHE	CG-CD1	5.32	1.46	1.38
1	A	855	VAL	CB-CG2	5.31	1.64	1.52
1	A	408	GLU	CB-CG	5.30	1.62	1.52
1	A	79	TYR	CD2-CE2	5.30	1.47	1.39
1	A	369	TYR	CD1-CE1	-5.29	1.31	1.39
1	A	204	GLN	CD-NE2	5.27	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ALA	CA-CB	5.27	1.63	1.52
1	A	718	LYS	CE-NZ	5.26	1.62	1.49
1	A	369	TYR	CE1-CZ	-5.25	1.31	1.38
1	A	781	TYR	CD2-CE2	5.25	1.47	1.39
1	A	352	SER	CA-CB	5.16	1.60	1.52
1	A	712	TYR	CD1-CE1	5.15	1.47	1.39
1	A	120	TYR	CB-CG	-5.13	1.44	1.51
1	A	553	ARG	CG-CD	5.11	1.64	1.51
1	A	479	TYR	CG-CD1	5.03	1.45	1.39
1	A	94	ASP	CB-CG	5.01	1.62	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	545	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	886	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	379	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	107	ASP	CB-CG-OD1	8.57	126.01	118.30
1	A	802	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	A	634	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	284	VAL	CB-CA-C	-7.56	97.04	111.40
1	A	544	TYR	CG-CD2-CE2	-7.23	115.51	121.30
1	A	371	LEU	CB-CG-CD2	7.13	123.12	111.00
1	A	679	PHE	CB-CG-CD1	-6.86	116.00	120.80
1	A	83	PHE	CB-CG-CD2	6.78	125.55	120.80
1	A	108	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	A	379	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	401	GLU	OE1-CD-OE2	6.63	131.25	123.30
1	A	83	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	A	322	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	789	ARG	CA-CB-CG	-6.49	99.12	113.40
1	A	600	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	A	544	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	A	587	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	361	GLN	CA-CB-CG	-6.17	99.82	113.40
1	A	522	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	910	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	545	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	599	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	329	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	A	115	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	369	TYR	CG-CD2-CE2	-5.66	116.77	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	867	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	886	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	580	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	A	907	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	444	GLU	N-CA-C	-5.42	96.38	111.00
1	A	463	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	A	926	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	204	GLN	CB-CA-C	-5.17	100.07	110.40
1	A	871	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	101	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	89	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	480	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	A	381	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	781	TYR	CB-CG-CD1	-5.06	117.96	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	ALA	Peptide

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	7205	0	6881	117	1
2	A	800	0	0	33	4
All	All	8005	0	6881	117	5

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 8.

All (117) 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:A:573:LEU:CA	1:A:929:ARG:HH12	1.25	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:CG	1:A:929:ARG:NH2	1.85	1.39
1:A:573:LEU:HA	1:A:929:ARG:NH1	1.14	1.37
1:A:571:LEU:HG	1:A:929:ARG:NH2	1.34	1.33
1:A:573:LEU:CA	1:A:929:ARG:NH1	1.90	1.18
1:A:572:LEU:O	1:A:929:ARG:NH1	1.80	1.14
1:A:571:LEU:CD2	1:A:929:ARG:HH21	1.65	1.09
1:A:571:LEU:CD2	1:A:929:ARG:NH2	2.18	1.06
1:A:41:ASN:HB3	2:A:1784:HOH:O	1.55	1.06
1:A:571:LEU:HD21	1:A:929:ARG:HH21	1.24	1.03
1:A:573:LEU:N	1:A:929:ARG:HH12	1.58	1.02
1:A:651[A]:MET:HE2	2:A:1797:HOH:O	1.60	0.99
1:A:571:LEU:HG	1:A:929:ARG:HH22	0.88	0.98
1:A:573:LEU:HA	1:A:929:ARG:CZ	1.95	0.96
1:A:571:LEU:CG	1:A:929:ARG:HH21	1.62	0.96
1:A:268:THR:HG23	2:A:1794:HOH:O	1.69	0.93
1:A:469[A]:ARG:CG	1:A:515[A]:CYS:SG	2.57	0.92
1:A:257:LEU:CB	2:A:1793:HOH:O	2.17	0.91
1:A:469[A]:ARG:HG3	1:A:515[A]:CYS:SG	2.12	0.90
1:A:572:LEU:C	1:A:929:ARG:HH12	1.74	0.89
1:A:571:LEU:CD1	1:A:929:ARG:NH2	2.35	0.88
1:A:774:ASN:HD21	1:A:880:SER:H	1.18	0.87
1:A:312:GLU:HG2	2:A:1796:HOH:O	1.73	0.86
1:A:571:LEU:HD21	1:A:929:ARG:NH2	1.85	0.84
1:A:80:LYS:HD3	2:A:1789:HOH:O	1.76	0.84
1:A:339:ASN:HD21	1:A:365:THR:H	1.25	0.84
1:A:469[A]:ARG:HG2	1:A:515[A]:CYS:SG	2.17	0.83
1:A:572:LEU:C	1:A:929:ARG:NH1	2.34	0.81
1:A:571:LEU:CD1	1:A:929:ARG:HH21	1.95	0.80
1:A:623[B]:HIS:HD2	2:A:1362:HOH:O	1.65	0.80
1:A:80:LYS:CE	2:A:1789:HOH:O	2.31	0.79
1:A:651[B]:MET:HE2	2:A:1797:HOH:O	1.85	0.76
1:A:861:LYS:HE2	2:A:1578:HOH:O	1.84	0.75
1:A:571:LEU:CG	1:A:929:ARG:HH22	1.67	0.75
1:A:59:ARG:HD3	2:A:1785:HOH:O	1.86	0.74
1:A:80:LYS:HE2	2:A:1789:HOH:O	1.86	0.73
1:A:787:LYS:HE3	2:A:1403:HOH:O	1.89	0.72
1:A:608[A]:LYS:HE3	2:A:1777:HOH:O	1.89	0.72
1:A:571:LEU:HD11	1:A:929:ARG:NH2	2.04	0.71
1:A:503[B]:MET:HE1	2:A:1670:HOH:O	1.91	0.69
1:A:18:ASP:HB2	2:A:1612:HOH:O	1.95	0.67
1:A:861:LYS:CE	2:A:1578:HOH:O	2.39	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH1	1:A:68:ILE:HD11	2.11	0.65
1:A:718:LYS:HE3	1:A:907:ASP:OD2	1.98	0.64
1:A:571:LEU:HD11	1:A:929:ARG:HH21	1.62	0.63
1:A:80:LYS:CD	2:A:1789:HOH:O	2.37	0.63
1:A:413[A]:CYS:SG	1:A:459:MET:HB2	2.39	0.63
1:A:405:THR:HG21	1:A:465:ALA:HA	1.81	0.63
1:A:910:ASP:HB2	2:A:1782:HOH:O	1.98	0.63
1:A:806:ASP:HB2	1:A:858:ILE:HG23	1.82	0.62
1:A:572:LEU:O	1:A:929:ARG:CZ	2.47	0.61
1:A:503[B]:MET:CE	2:A:1670:HOH:O	2.48	0.57
1:A:719:LYS:HE2	1:A:905:GLU:OE2	2.06	0.56
1:A:41:ASN:CB	2:A:1784:HOH:O	2.32	0.55
1:A:59:ARG:CD	2:A:1785:HOH:O	2.49	0.54
1:A:401:GLU:OE2	2:A:1692:HOH:O	2.18	0.54
1:A:429:LYS:HE3	2:A:1776:HOH:O	2.07	0.54
1:A:534:PHE:CD1	1:A:710:THR:HB	2.43	0.54
1:A:725:ASP:O	1:A:726:SER:OG	2.20	0.53
1:A:890:ASN:ND2	1:A:892:LEU:H	2.07	0.53
1:A:539:ASN:HD22	1:A:539:ASN:C	2.12	0.52
1:A:608[A]:LYS:HG2	1:A:610:ASP:OD1	2.09	0.52
1:A:415:PRO:HD3	1:A:457:PHE:O	2.10	0.52
1:A:608[A]:LYS:CE	2:A:1777:HOH:O	2.53	0.52
1:A:670:ASN:ND2	1:A:672:ALA:H	2.09	0.51
1:A:374:ASP:OD2	1:A:790[A]:MET:HB3	2.10	0.51
1:A:499:THR:O	1:A:503[B]:MET:HG3	2.09	0.51
1:A:569:LYS:NZ	1:A:570:ASN:HD21	2.08	0.51
1:A:419:VAL:HG21	1:A:452:ARG:CB	2.41	0.50
1:A:369:TYR:OH	2:A:1368:HOH:O	2.17	0.49
1:A:497:PRO:HA	1:A:502:TYR:CD1	2.47	0.49
1:A:183:ILE:HD13	1:A:219:ALA:HB2	1.93	0.49
1:A:352:SER:HB2	2:A:1774:HOH:O	2.13	0.49
1:A:339:ASN:ND2	1:A:365:THR:H	2.02	0.49
1:A:684:THR:HG22	1:A:914:LEU:HG	1.95	0.49
1:A:355:ASN:HD22	1:A:356:ALA:N	2.11	0.48
1:A:861:LYS:NZ	2:A:1578:HOH:O	2.48	0.47
1:A:17:GLN:HB3	1:A:21:GLU:HB2	1.96	0.47
1:A:806:ASP:CB	1:A:858:ILE:HG23	2.43	0.47
1:A:442:ALA:O	1:A:443:THR:C	2.53	0.47
1:A:666:ILE:HD12	1:A:666:ILE:N	2.31	0.46
1:A:355:ASN:ND2	1:A:357:VAL:H	2.13	0.46
1:A:178:ILE:HG12	1:A:183:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASP:HA	1:A:539:ASN:HD21	1.81	0.45
1:A:861:LYS:NZ	2:A:1530:HOH:O	2.27	0.45
1:A:890:ASN:HD22	1:A:892:LEU:H	1.63	0.45
1:A:608[A]:LYS:CG	1:A:610:ASP:OD1	2.65	0.45
1:A:785[A]:SER:HB3	1:A:795:ARG:HH22	1.82	0.45
1:A:861:LYS:HE3	2:A:1469:HOH:O	2.16	0.44
1:A:371:LEU:HD22	1:A:791:TYR:CD2	2.53	0.44
1:A:539:ASN:ND2	1:A:542:LEU:H	2.15	0.44
1:A:573:LEU:C	1:A:929:ARG:NH1	2.63	0.44
1:A:199:PHE:CD1	1:A:243:ASN:HB3	2.53	0.44
1:A:802:ARG:CZ	1:A:804:VAL:HG11	2.48	0.43
1:A:80:LYS:HD2	1:A:581:GLU:OE2	2.18	0.43
1:A:574:LEU:N	1:A:929:ARG:NH1	2.66	0.43
1:A:744:ILE:HG12	1:A:764:TRP:CE2	2.54	0.43
1:A:379:ARG:HB2	1:A:790[B]:MET:SD	2.59	0.43
1:A:259:SER:OG	1:A:261:VAL:HG23	2.19	0.42
1:A:522:ARG:HH22	1:A:798:GLN:NE2	2.17	0.42
1:A:891:LEU:HD12	2:A:1757:HOH:O	2.18	0.42
1:A:331:ASN:HD21	1:A:388:GLN:HG3	1.84	0.42
1:A:574:LEU:HG	1:A:929:ARG:HD2	2.02	0.42
1:A:176:ILE:HD12	1:A:186:GLY:HA2	2.02	0.42
1:A:339:ASN:O	1:A:361:GLN:HG2	2.20	0.42
1:A:495:ASP:OD2	2:A:1682:HOH:O	2.22	0.41
1:A:787:LYS:CE	2:A:1403:HOH:O	2.58	0.41
1:A:196:ASP:C	1:A:196:ASP:OD1	2.58	0.41
1:A:464:ASN:HD22	1:A:464:ASN:HA	1.62	0.41
1:A:179:THR:OG1	1:A:181:GLU:HB2	2.20	0.41
1:A:173:TYR:O	1:A:218:ALA:HA	2.21	0.41
1:A:66:ARG:HH12	1:A:68:ILE:HD11	1.83	0.41
1:A:176:ILE:CD1	1:A:186:GLY:HA2	2.50	0.41
1:A:337:TYR:CZ	1:A:585:ARG:HG2	2.56	0.41
1:A:444:GLU:HG2	1:A:445:PHE:HD1	1.86	0.41
1:A:53:HIS:HD2	1:A:54:ASP:OD1	2.04	0.40
1:A:81:ALA:O	1:A:581:GLU:HA	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:NE2	1:A:821:GLN:O[2_555]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1764:HOH:O	2:A:1767:HOH:O[2_555]	1.79	0.41
2:A:1426:HOH:O	2:A:1764:HOH:O[3_555]	1.92	0.28
2:A:1623:HOH:O	2:A:1764:HOH:O[3_555]	2.07	0.13
2:A:1554:HOH:O	2:A:1717:HOH:O[3_555]	2.19	0.01

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	891/951 (94%)	855 (96%)	32 (4%)	4 (0%)	34 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	GLU
1	A	214	GLU
1	A	443	THR
1	A	776	GLY

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	783/828 (95%)	765 (98%)	18 (2%)	50 23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	THR
1	A	209	GLN
1	A	213	THR
1	A	226	THR
1	A	352	SER
1	A	354	LEU
1	A	355	ASN
1	A	427	LYS
1	A	443	THR
1	A	489	SER
1	A	539	ASN
1	A	577	SER
1	A	608[A]	LYS
1	A	608[B]	LYS
1	A	665	SER
1	A	749	ASP
1	A	836	ARG
1	A	896	SER

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	53	HIS
1	A	61	GLN
1	A	264	GLN
1	A	331	ASN
1	A	339	ASN
1	A	355	ASN
1	A	370	GLN
1	A	388	GLN
1	A	464	ASN
1	A	470	ASN
1	A	539	ASN
1	A	570	ASN
1	A	670	ASN
1	A	774	ASN
1	A	798	GLN
1	A	890	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	889/951 (93%)	-0.36	20 (2%) 62 63	13, 22, 47, 68	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	ILE	5.7
1	A	7	PRO	5.0
1	A	443	THR	4.6
1	A	257	LEU	4.3
1	A	895	ASN	3.8
1	A	191	THR	3.3
1	A	279	LEU	3.3
1	A	269	THR	3.1
1	A	307	GLU	2.9
1	A	891	LEU	2.9
1	A	187	VAL	2.6
1	A	211	TYR	2.6
1	A	946	ALA	2.5
1	A	444	GLU	2.5
1	A	929	ARG	2.5
1	A	212	GLU	2.4
1	A	280	THR	2.1
1	A	213	THR	2.1
1	A	445	PHE	2.1
1	A	250	VAL	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.