Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:56 AM GMT

PDB ID	:	2EWF
Title	:	Crystal structure of the site-specific DNA nickase N.BspD6I
Authors	:	Kachalova, G.S.; Bartunik, H.D.; Artyukh, R.I.; Rogulin, E.A.; Perevyazova, T.A.; Zheleznaya, L.A.; Matvienko, N.I.
Deposited on	:	2005-11-03
Resolution	:	1.84 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

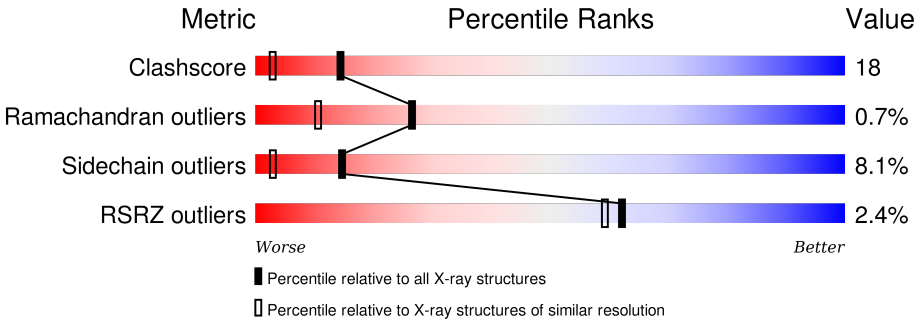
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.84 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))
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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. 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	610	2% 67% 24% 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	605	-	-	X	-
2	BR	A	614	-	-	X	X
2	BR	A	616	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5517 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 Nicking endonuclease N.BspD6I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	2	0
			4872	3132	824	900	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8GCA3
A	-4	HIS	-	EXPRESSION TAG	UNP Q8GCA3
A	-3	HIS	-	EXPRESSION TAG	UNP Q8GCA3
A	-2	HIS	-	EXPRESSION TAG	UNP Q8GCA3
A	-1	HIS	-	EXPRESSION TAG	UNP Q8GCA3
A	0	HIS	-	EXPRESSION TAG	UNP Q8GCA3

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	Br	0	0
			13	13		

- Molecule 3 is water.

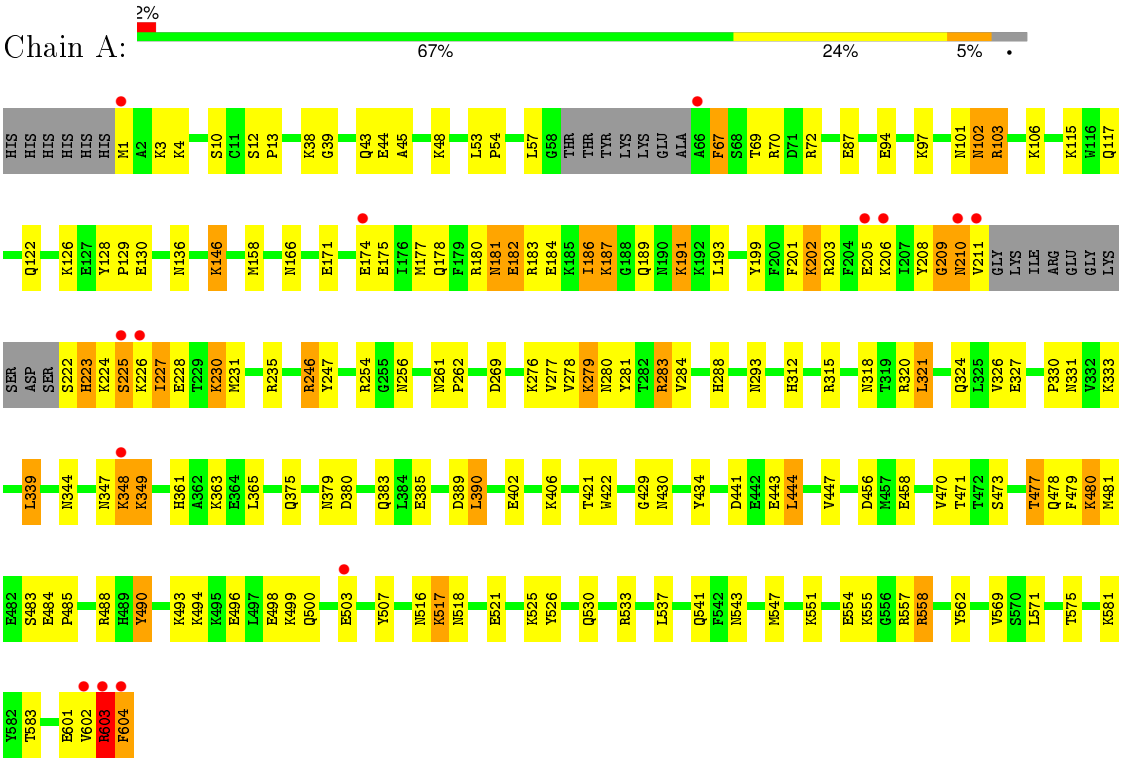
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	627	Total	O	0	5
			632	632		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Nicking endonuclease N.BspD6I

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.55Å 92.56Å 76.35Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	10.00 – 1.84 19.78 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-1.84) 95.6 (19.78-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 1.84Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.183 , 0.236 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 89.5	EDS
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 66483 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5517	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BR

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	0.37	0/4969	1.03	18/6687 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	488	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	103	ARG	NE-CZ-NH2	9.38	124.99	120.30
1	A	488	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	A	558	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	246	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	380	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	558	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	283	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	456	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	283	ARG	CD-NE-CZ	-5.88	115.37	123.60
1	A	441	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	562	TYR	CB-CG-CD2	5.69	124.42	121.00
1	A	562	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	422	TRP	CA-CB-CG	5.57	124.29	113.70
1	A	490	TYR	CG-CD1-CE1	5.56	125.75	121.30
1	A	199	TYR	CB-CG-CD1	5.25	124.15	121.00
1	A	281	TYR	CB-CG-CD2	5.15	124.09	121.00
1	A	103	ARG	NE-CZ-NH1	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4872	0	4916	174	0
2	A	13	0	0	9	0
3	A	632	0	0	42	0
All	All	5517	0	4916	176	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 18.

All (176) 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:603:ARG:H	1:A:603:ARG:CD	1.31	1.35
1:A:603:ARG:HD3	1:A:603:ARG:N	1.51	1.19
1:A:210:ASN:O	1:A:211:VAL:HG23	1.46	1.16
1:A:97:LYS:HE2	3:A:2609:HOH:O	1.42	1.14
1:A:603:ARG:HH11	1:A:603:ARG:HG2	1.16	1.07
1:A:222:SER:N	1:A:226:LYS:HZ3	1.58	1.00
1:A:603:ARG:HH11	1:A:603:ARG:CG	1.80	0.94
1:A:339:LEU:HD22	1:A:365:LEU:HD23	1.52	0.90
1:A:603:ARG:HD3	1:A:603:ARG:H	0.69	0.86
1:A:331:ASN:HD21	1:A:375:GLN:HE22	1.26	0.84
2:A:606:BR:BR	3:A:2445:HOH:O	2.51	0.84
1:A:603:ARG:CD	1:A:603:ARG:N	2.12	0.83
1:A:97:LYS:CE	3:A:2609:HOH:O	2.13	0.82
1:A:117:GLN:HE22	1:A:278:VAL:H	1.27	0.82
1:A:187:LYS:HD2	3:A:2091:HOH:O	1.86	0.76
1:A:494:LYS:O	1:A:498:GLU:HG3	1.86	0.76
1:A:101:ASN:HD22	1:A:103:ARG:HH12	1.33	0.75
1:A:254:ARG:HG3	3:A:2219:HOH:O	1.87	0.74
1:A:203[B]:ARG:HG3	3:A:2370:HOH:O	1.87	0.72
1:A:45:ALA:HA	1:A:48:LYS:HE2	1.71	0.72
1:A:477:THR:O	1:A:480:LYS:HB3	1.89	0.72
1:A:478:GLN:HE22	1:A:516:ASN:H	1.39	0.71
1:A:348:LYS:HB2	1:A:349:LYS:HD3	1.73	0.70
1:A:390:LEU:HD13	3:A:2332:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:O	1:A:211:VAL:CG2	2.33	0.67
1:A:320:ARG:O	1:A:324:GLN:HG3	1.94	0.67
1:A:183:ARG:NH1	2:A:617:BR:BR	2.83	0.66
1:A:348:LYS:H	1:A:348:LYS:HD2	1.59	0.66
1:A:601:GLU:OE1	3:A:2685:HOH:O	2.14	0.65
1:A:191:LYS:HD3	2:A:605:BR:BR	2.52	0.65
1:A:318:ASN:HB3	1:A:339:LEU:HD21	1.79	0.64
1:A:177:MET:HE1	3:A:2456:HOH:O	1.97	0.64
1:A:344:ASN:O	1:A:347:ASN:HB2	1.97	0.64
1:A:402:GLU:O	1:A:406:LYS:HG3	1.99	0.63
1:A:478:GLN:NE2	1:A:516:ASN:H	1.97	0.63
1:A:189:GLN:HE21	1:A:193:LEU:HD21	1.63	0.63
1:A:479:PHE:HD1	1:A:483:SER:HG	1.48	0.62
1:A:189:GLN:NE2	1:A:193:LEU:HD21	2.14	0.62
1:A:130:GLU:HG3	3:A:2266:HOH:O	1.99	0.62
1:A:603:ARG:CG	1:A:603:ARG:NH1	2.47	0.61
1:A:222:SER:O	1:A:223:HIS:C	2.37	0.61
1:A:517:LYS:O	1:A:521:GLU:HG3	2.01	0.61
1:A:222:SER:O	1:A:226:LYS:HG2	2.01	0.60
1:A:10:SER:HA	3:A:2342:HOH:O	2.00	0.60
1:A:603:ARG:NH1	1:A:603:ARG:HG2	1.98	0.60
1:A:604:PHE:HB3	3:A:2447:HOH:O	2.01	0.60
1:A:223:HIS:O	1:A:226:LYS:N	2.27	0.60
1:A:1:MET:HG2	1:A:3:LYS:HD3	1.84	0.59
1:A:101:ASN:ND2	1:A:103:ARG:HH12	2.00	0.59
1:A:603:ARG:HD2	1:A:603:ARG:H	1.53	0.59
1:A:126:LYS:HG2	3:A:2672:HOH:O	2.02	0.59
1:A:202:LYS:O	1:A:205:GLU:HB3	2.03	0.59
1:A:186:ILE:CG2	1:A:191:LYS:HB3	2.33	0.59
1:A:177:MET:HE2	1:A:177:MET:HA	1.86	0.58
1:A:94:GLU:HG3	3:A:2283:HOH:O	2.05	0.57
1:A:45:ALA:HA	1:A:48:LYS:CE	2.35	0.57
1:A:496:GLU:O	1:A:500:GLN:HG3	2.05	0.57
1:A:312:HIS:HD2	3:A:2156:HOH:O	1.87	0.56
1:A:54:PRO:HA	1:A:57:LEU:HD12	1.86	0.56
1:A:227:ILE:O	1:A:231:MET:HG3	2.05	0.56
1:A:516:ASN:HD21	1:A:518:ASN:HB2	1.69	0.56
1:A:555:LYS:HG3	1:A:603:ARG:HH21	1.69	0.56
1:A:101:ASN:HD22	1:A:103:ARG:NH1	2.00	0.56
1:A:177:MET:CE	1:A:180:ARG:HD2	2.36	0.55
1:A:174:GLU:HA	1:A:174:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:MET:HB3	3:A:2360:HOH:O	2.06	0.55
1:A:477:THR:HA	1:A:480:LYS:HB3	1.89	0.55
1:A:201:PHE:CZ	1:A:224:LYS:HG3	2.43	0.54
1:A:480:LYS:HE3	1:A:481:MET:CA	2.37	0.54
1:A:39:GLY:O	1:A:43:GLN:HG3	2.07	0.54
1:A:4:LYS:HG3	1:A:128:TYR:CZ	2.43	0.54
1:A:330:PRO:HD2	2:A:613:BR:BR	2.62	0.54
1:A:555:LYS:HD2	1:A:603:ARG:HE	1.73	0.53
1:A:203[B]:ARG:HG2	3:A:2228:HOH:O	2.09	0.53
1:A:191:LYS:HE3	2:A:605:BR:BR	2.64	0.53
1:A:208:TYR:C	1:A:210:ASN:N	2.62	0.53
2:A:614:BR:BR	3:A:2044:HOH:O	2.74	0.53
1:A:551:LYS:HG2	1:A:603:ARG:NH1	2.24	0.53
1:A:187:LYS:HA	3:A:2091:HOH:O	2.07	0.52
1:A:443:GLU:O	1:A:444:LEU:HB2	2.08	0.52
1:A:481:MET:HG3	3:A:2460:HOH:O	2.08	0.52
1:A:477:THR:HG22	3:A:2078:HOH:O	2.10	0.52
1:A:318:ASN:CB	1:A:339:LEU:HD21	2.39	0.52
1:A:361:HIS:HD2	3:A:2383[B]:HOH:O	1.92	0.51
1:A:177:MET:HE1	1:A:180:ARG:HD2	1.92	0.51
1:A:421:THR:HG21	1:A:470:VAL:HG11	1.93	0.51
1:A:117:GLN:NE2	1:A:278:VAL:H	2.04	0.50
1:A:471:THR:OG1	1:A:473:SER:HB2	2.11	0.50
1:A:537:LEU:HD22	1:A:541:GLN:HB3	1.93	0.50
1:A:223:HIS:HE1	3:A:2333:HOH:O	1.94	0.50
1:A:126:LYS:HD2	3:A:2087:HOH:O	2.11	0.49
1:A:280:ASN:ND2	1:A:280:ASN:H	2.11	0.49
1:A:507:TYR:OH	1:A:569:VAL:HG22	2.12	0.49
1:A:277:VAL:O	1:A:279:LYS:HE3	2.13	0.48
1:A:603:ARG:HD2	1:A:603:ARG:N	2.15	0.48
1:A:103:ARG:HD2	3:A:2337:HOH:O	2.14	0.48
1:A:480:LYS:HE3	1:A:481:MET:N	2.29	0.48
1:A:53:LEU:O	1:A:57:LEU:HG	2.14	0.48
1:A:344:ASN:C	1:A:348:LYS:HZ2	2.18	0.47
1:A:458:GLU:OE2	1:A:493:LYS:HE2	2.14	0.47
1:A:477:THR:O	1:A:481:MET:HB2	2.14	0.47
1:A:209:GLY:O	1:A:210:ASN:O	2.32	0.47
1:A:187:LYS:HA	1:A:187:LYS:HD2	1.77	0.47
1:A:136:ASN:HD22	1:A:166:ASN:HD21	1.62	0.46
1:A:222:SER:HB3	1:A:225:SER:HB3	1.95	0.46
1:A:191:LYS:CE	2:A:605:BR:BR	3.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLU:HB3	1:A:485:PRO:HD3	1.97	0.46
1:A:555:LYS:CE	1:A:603:ARG:HE	2.28	0.46
1:A:208:TYR:O	1:A:210:ASN:N	2.49	0.46
1:A:490:TYR:OH	1:A:533:ARG:HG3	2.16	0.45
1:A:158:MET:O	1:A:203[B]:ARG:NH2	2.50	0.45
1:A:208:TYR:C	1:A:210:ASN:H	2.18	0.45
1:A:146:LYS:NZ	1:A:269:ASP:OD1	2.50	0.45
1:A:38:LYS:HB2	1:A:38:LYS:HE3	1.63	0.45
1:A:551:LYS:O	1:A:603:ARG:NH2	2.50	0.45
1:A:205:GLU:HG3	3:A:2333:HOH:O	2.15	0.45
1:A:12:SER:HB3	1:A:72:ARG:NH1	2.31	0.45
1:A:571:LEU:O	1:A:575:THR:HG23	2.16	0.45
1:A:87:GLU:OE1	1:A:87:GLU:N	2.50	0.45
1:A:344:ASN:ND2	3:A:2433:HOH:O	2.50	0.45
1:A:349:LYS:HD3	1:A:349:LYS:N	2.31	0.45
1:A:146:LYS:NZ	3:A:2549:HOH:O	2.50	0.45
1:A:122:GLN:NE2	3:A:2459:HOH:O	2.50	0.45
1:A:383:GLN:NE2	3:A:2374:HOH:O	2.50	0.45
1:A:201:PHE:CE2	1:A:224:LYS:HG3	2.52	0.45
1:A:181:ASN:HA	1:A:181:ASN:HD22	1.45	0.45
1:A:246:ARG:CZ	1:A:447:VAL:HG22	2.46	0.45
1:A:349:LYS:O	1:A:349:LYS:HG2	2.17	0.44
1:A:182:GLU:OE2	1:A:182:GLU:N	2.50	0.44
1:A:375:GLN:NE2	1:A:434:TYR:OH	2.50	0.44
1:A:70:ARG:NH2	3:A:2662:HOH:O	2.50	0.44
1:A:283:ARG:NE	3:A:2555:HOH:O	2.50	0.44
1:A:106:LYS:NZ	3:A:2363:HOH:O	2.50	0.44
1:A:363:LYS:NZ	3:A:2020:HOH:O	2.50	0.44
1:A:115:LYS:NZ	1:A:293:ASN:O	2.50	0.44
1:A:175[A]:GLU:O	1:A:175[A]:GLU:HG2	2.18	0.44
1:A:555:LYS:CD	1:A:603:ARG:HE	2.31	0.44
1:A:279:LYS:NZ	3:A:2547:HOH:O	2.50	0.44
1:A:201:PHE:CE2	1:A:227:ILE:HG12	2.53	0.44
1:A:235:ARG:NH2	3:A:2557:HOH:O	2.51	0.44
1:A:326:VAL:HG22	1:A:326:VAL:O	2.18	0.44
1:A:421:THR:HG21	1:A:470:VAL:CG1	2.49	0.43
1:A:477:THR:C	1:A:480:LYS:HB3	2.38	0.43
1:A:122:GLN:HG2	3:A:2459:HOH:O	2.17	0.43
1:A:224:LYS:HE3	1:A:228:GLU:OE2	2.18	0.43
1:A:235:ARG:NH1	3:A:2285:HOH:O	2.50	0.43
1:A:261:ASN:HA	1:A:262:PRO:HD2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:MET:HE3	3:A:2531:HOH:O	2.19	0.43
1:A:429:GLY:O	1:A:430:ASN:HB2	2.19	0.43
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.46	0.43
1:A:223:HIS:O	1:A:224:LYS:C	2.56	0.42
1:A:175[A]:GLU:HG3	3:A:2118:HOH:O	2.20	0.42
1:A:256:ASN:ND2	3:A:2508:HOH:O	2.50	0.42
1:A:554:GLU:HB2	1:A:603:ARG:HH22	1.83	0.42
1:A:70:ARG:HG2	1:A:70:ARG:HH11	1.84	0.42
1:A:284:VAL:O	1:A:288:HIS:HD2	2.02	0.42
1:A:379:ASN:OD1	1:A:558:ARG:NH2	2.49	0.41
1:A:279:LYS:HD3	1:A:279:LYS:HA	1.76	0.41
1:A:117:GLN:HE22	1:A:278:VAL:HG22	1.85	0.41
1:A:191:LYS:CD	2:A:605:BR:BR	3.23	0.41
1:A:70:ARG:NH1	1:A:70:ARG:HG2	2.35	0.41
1:A:102:ASN:HA	1:A:102:ASN:HD22	1.54	0.41
1:A:223:HIS:HA	1:A:226:LYS:HG3	2.03	0.41
1:A:186:ILE:HD13	1:A:186:ILE:N	2.36	0.41
1:A:186:ILE:HG22	1:A:191:LYS:HB3	2.01	0.41
1:A:385:GLU:OE2	1:A:389:ASP:OD1	2.38	0.41
1:A:126:LYS:O	1:A:129:PRO:HD3	2.21	0.41
1:A:473:SER:HB2	1:A:481:MET:CE	2.51	0.41
1:A:344:ASN:HA	1:A:344:ASN:HD22	1.71	0.41
1:A:321:LEU:HA	1:A:321:LEU:HD12	1.88	0.41
1:A:177:MET:CA	1:A:177:MET:HE2	2.51	0.41
1:A:247:TYR:HA	2:A:614:BR:BR	2.76	0.41
1:A:477:THR:HA	1:A:480:LYS:CB	2.51	0.40
1:A:526:TYR:CD2	1:A:530:GLN:HG3	2.56	0.40
1:A:136:ASN:ND2	1:A:166:ASN:HD21	2.19	0.40
1:A:67:PHE:HE1	3:A:2113:HOH:O	2.04	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	582/610 (95%)	564 (97%)	14 (2%)	4 (1%)	26 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	223	HIS
1	A	603	ARG
1	A	209	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	535/554 (97%)	492 (92%)	43 (8%)	15 3

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	44	GLU
1	A	67	PHE
1	A	69	THR
1	A	102	ASN
1	A	146	LYS
1	A	171	GLU
1	A	178	GLN
1	A	181	ASN
1	A	182	GLU
1	A	184	GLU
1	A	186	ILE
1	A	187	LYS
1	A	191	LYS
1	A	202	LYS
1	A	206	LYS
1	A	225	SER

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Mol	Chain	Res	Type
1	A	227	ILE
1	A	230	LYS
1	A	276	LYS
1	A	279	LYS
1	A	315	ARG
1	A	321	LEU
1	A	327	GLU
1	A	333	LYS
1	A	339	LEU
1	A	348	LYS
1	A	349	LYS
1	A	390	LEU
1	A	444	LEU
1	A	477	THR
1	A	480	LYS
1	A	499	LYS
1	A	503	GLU
1	A	517	LYS
1	A	525	LYS
1	A	543	ASN
1	A	557	ARG
1	A	581	LYS
1	A	583	THR
1	A	602	VAL
1	A	603	ARG
1	A	604	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	102	ASN
1	A	117	GLN
1	A	123	HIS
1	A	136	ASN
1	A	181	ASN
1	A	189	GLN
1	A	210	ASN
1	A	257	GLN
1	A	280	ASN
1	A	288	HIS
1	A	312	HIS

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Mol	Chain	Res	Type
1	A	366	GLN
1	A	375	GLN
1	A	478	GLN
1	A	516	ASN
1	A	543	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	587/610 (96%)	-0.13	14 (2%) 62 59	20, 33, 58, 81	21 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	ASN	10.0
1	A	604	PHE	7.1
1	A	211	VAL	6.4
1	A	1	MET	4.2
1	A	66	ALA	4.2
1	A	603	ARG	4.0
1	A	226	LYS	3.7
1	A	602	VAL	3.5
1	A	174	GLU	2.7
1	A	503	GLU	2.7
1	A	205	GLU	2.5
1	A	206	LYS	2.5
1	A	225	SER	2.2
1	A	348	LYS	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BR	A	614	1/1	0.98	0.14	4.32	54,54,54,54	0
2	BR	A	616	1/1	0.98	0.14	3.49	53,53,53,53	1
2	BR	A	612	1/1	1.00	0.04	-1.27	57,57,57,57	0
2	BR	A	609	1/1	1.00	0.04	-2.60	51,51,51,51	0
2	BR	A	610	1/1	0.99	0.04	-2.84	47,47,47,47	0
2	BR	A	607	1/1	0.99	0.03	-2.98	40,40,40,40	0
2	BR	A	605	1/1	0.99	0.03	-3.31	44,44,44,44	0
2	BR	A	615	1/1	0.99	0.04	-	54,54,54,54	0
2	BR	A	617	1/1	0.97	0.04	-	51,51,51,51	1
2	BR	A	611	1/1	1.00	0.02	-	39,39,39,39	1
2	BR	A	608	1/1	0.99	0.06	-	55,55,55,55	0
2	BR	A	606	1/1	1.00	0.02	-	36,36,36,36	0
2	BR	A	613	1/1	0.97	0.08	-	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.