



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 2EWF / pdb_00002ewf
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

<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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

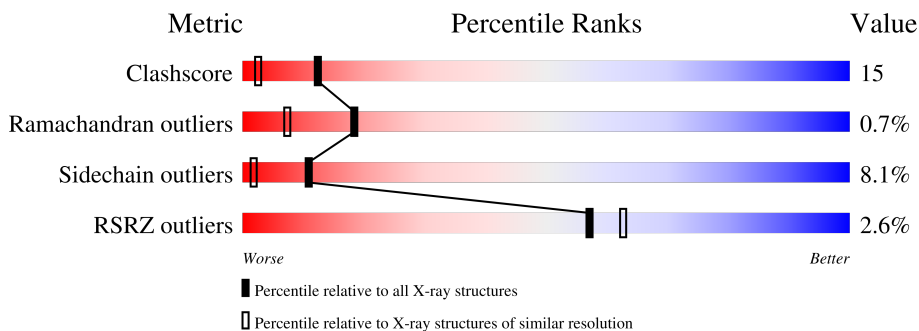
1 Overall quality at a glance

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	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 $\leq 5\%$. 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	

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	-

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
			Total	C	N	O	S			
1	A	587	4872	3132	824	900	16	0	2	0

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 (CCD ID: BR) (formula: Br).

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

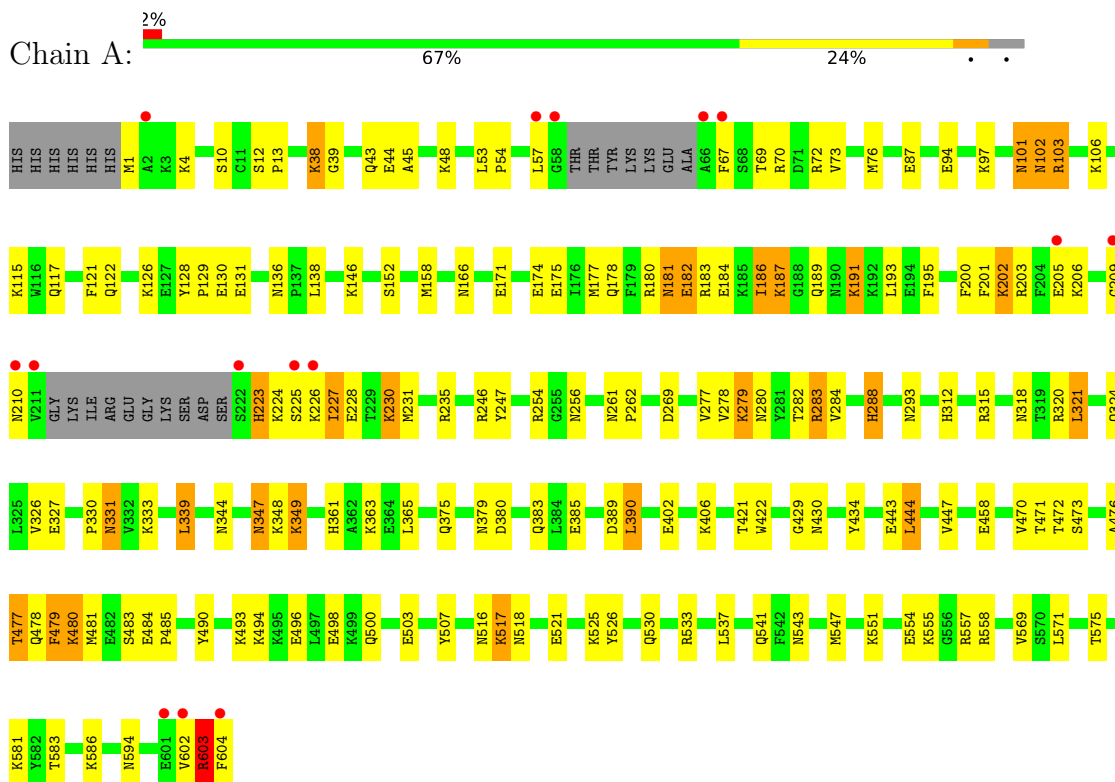
- Molecule 3 is water.

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

3 Residue-property plots

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: Nicking endonuclease N.BspD6I



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 10.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-1.84) 95.0 (10.00-1.84)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.84Å)	Xtrriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.183 , 0.236 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtrriage
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

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

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	0.46	0/4969	1.32	21/6687 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	SER	CA-C-O	-6.61	114.34	121.94
1	A	283	ARG	CD-NE-CZ	-6.45	115.37	124.40
1	A	103	ARG	NE-CZ-NH2	6.43	124.99	119.20
1	A	479	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	200	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	101	ASN	CA-CB-CG	-5.87	106.73	112.60
1	A	288	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	195	PHE	CA-CB-CG	5.86	119.66	113.80
1	A	380	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	331	ASN	CA-CB-CG	5.73	118.33	112.60
1	A	347	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	422	TRP	CA-CB-CG	5.63	124.29	113.60
1	A	594	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	138	LEU	CA-C-O	5.35	126.10	120.42
1	A	121	PHE	CA-CB-CG	-5.26	108.53	113.80
1	A	476	ALA	CA-C-N	-5.21	112.02	120.72
1	A	476	ALA	C-N-CA	-5.21	112.02	120.72
1	A	282	THR	CA-C-N	-5.19	115.15	122.94
1	A	282	THR	C-N-CA	-5.19	115.15	122.94
1	A	472	THR	CA-C-N	5.08	128.28	120.82
1	A	472	THR	C-N-CA	5.08	128.28	120.82

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	4872	0	4916	149	0
2	A	13	0	0	9	0
3	A	632	0	0	39	0
All	All	5517	0	4916	151	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 15.

All (151) 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:339:LEU:HD22	1:A:365:LEU:HD23	1.52	0.90
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: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:177:MET:HE1	3:A:2456:HOH:O	1.86	0.73
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
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:HD2	1:A:348:LYS:H	1.59	0.66
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: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:189:GLN:HE21	1:A:193:LEU:HD21	1.63	0.63
1:A:478:GLN:NE2	1:A:516:ASN:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:HD1	1:A:483:SER:HG	1.48	0.62
1:A:130:GLU:HG3	3:A:2266:HOH:O	1.99	0.62
1:A:189:GLN:NE2	1:A:193:LEU:HD21	2.14	0.62
1:A:517:LYS:O	1:A:521:GLU:HG3	2.01	0.61
1:A:10:SER:HA	3:A:2342:HOH:O	2.00	0.60
1:A:177:MET:HA	1:A:177:MET:HE2	1.83	0.60
1:A:604:PHE:HB3	3:A:2447:HOH:O	2.01	0.60
1:A:101:ASN:ND2	1:A:103:ARG:HH12	2.00	0.59
1:A:126:LYS:HG2	3:A:2672:HOH:O	2.02	0.59
1:A:186:ILE:CG2	1:A:191:LYS:HB3	2.33	0.59
1:A:202:LYS:O	1:A:205:GLU:HB3	2.03	0.59
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:177:MET:HE1	1:A:180:ARG:HH11	1.69	0.57
1:A:54:PRO:HA	1:A:57:LEU:HD12	1.86	0.56
1:A:312:HIS:HD2	3:A:2156:HOH:O	1.87	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
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:4:LYS:HG3	1:A:128:TYR:CZ	2.43	0.54
1:A:39:GLY:O	1:A:43:GLN:HG3	2.07	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
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:177:MET:HE2	1:A:180:ARG:HD2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:HIS:HD2	3:A:2383[B]:HOH:O	1.92	0.51
1:A:421:THR:HG21	1:A:470:VAL:HG11	1.93	0.51
1:A:344:ASN:C	1:A:348:LYS:HZ2	2.19	0.50
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: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:280:ASN:ND2	1:A:280:ASN:H	2.11	0.48
1:A:477:THR:C	1:A:480:LYS:HB3	2.38	0.48
1:A:103:ARG:HD2	3:A:2337:HOH:O	2.14	0.48
1:A:53:LEU:O	1:A:57:LEU:HG	2.14	0.48
1:A:480:LYS:HE3	1:A:481:MET:N	2.29	0.48
1:A:473:SER:HB2	1:A:481:MET:HE2	1.96	0.48
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:187:LYS:HD2	1:A:187:LYS:HA	1.77	0.47
1:A:136:ASN:HD22	1:A:166:ASN:HD21	1.62	0.46
1:A:191:LYS:CE	2:A:605:BR:BR	3.19	0.46
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:490:TYR:OH	1:A:533:ARG:HG3	2.16	0.45
1:A:73:VAL:HA	1:A:76:MET:HE3	1.98	0.45
1:A:158:MET:O	1:A:203[B]:ARG:NH2	2.50	0.45
1:A:38:LYS:HE3	1:A:38:LYS:HB2	1.63	0.45
1:A:146:LYS:NZ	1:A:269:ASP:OD1	2.50	0.45
1:A:12:SER:HB3	1:A:72:ARG:NH1	2.31	0.45
1:A:87:GLU:OE1	1:A:87:GLU:N	2.50	0.45
1:A:205:GLU:HG3	3:A:2333:HOH:O	2.15	0.45
1:A:551:LYS:O	1:A:603:ARG:NH2	2.50	0.45
1:A:571:LEU:O	1:A:575:THR:HG23	2.16	0.45
1:A:126:LYS:NZ	3:A:2087:HOH:O	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:122:GLN:NE2	3:A:2459:HOH:O	2.50	0.45
1:A:146:LYS:NZ	3:A:2549:HOH:O	2.50	0.45
1:A:383:GLN:NE2	3:A:2374:HOH:O	2.50	0.45
1:A:181:ASN:HD22	1:A:181:ASN:HA	1.45	0.45
1:A:201:PHE:CE2	1:A:224:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:CZ	1:A:447:VAL:HG22	2.46	0.45
1:A:182:GLU:N	1:A:182:GLU:OE2	2.50	0.44
1:A:349:LYS:O	1:A:349:LYS:HG2	2.17	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:375:GLN:NE2	1:A:434:TYR:OH	2.50	0.44
1:A:106:LYS:NZ	3:A:2363:HOH:O	2.50	0.44
1:A:115:LYS:NZ	1:A:293:ASN:O	2.50	0.44
1:A:363:LYS:NZ	3:A:2020:HOH:O	2.50	0.44
1:A:175[A]:GLU:O	1:A:175[A]:GLU:HG2	2.18	0.44
1:A:279:LYS:NZ	3:A:2547:HOH:O	2.50	0.44
1:A:555:LYS:CD	1:A:603:ARG:HE	2.31	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:O	1:A:326:VAL:HG22	2.18	0.44
1:A:421:THR:HG21	1:A:470:VAL:CG1	2.49	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
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.46	0.43
1:A:429:GLY:O	1:A:430:ASN:HB2	2.19	0.43
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:HA	1:A:279:LYS:HD3	1.76	0.41
1:A:70:ARG:HG2	1:A:70:ARG:NH1	2.35	0.41
1:A:102:ASN:HD22	1:A:102:ASN:HA	1.54	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:186:ILE:N	1:A:186:ILE:HD13	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:321:LEU:HD12	1:A:321:LEU:HA	1.88	0.41
1:A:344:ASN:HD22	1:A:344:ASN:HA	1.71	0.41
1:A:473:SER:HB2	1:A:481:MET:CE	2.51	0.41
1:A:247:TYR:HA	2:A:614:BR:BR	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18 7

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%)	11 2

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	PRO
1	A	38	LYS
1	A	44	GLU
1	A	69	THR
1	A	97	LYS
1	A	102	ASN
1	A	131	GLU
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
1	A	226	LYS
1	A	227	ILE
1	A	230	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	349	LYS
1	A	390	LEU
1	A	444	LEU
1	A	477	THR
1	A	480	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	586	LYS
1	A	602	VAL

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Mol	Chain	Res	Type
1	A	603	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	198	ASN
1	A	210	ASN
1	A	257	GLN
1	A	280	ASN
1	A	288	HIS
1	A	312	HIS
1	A	375	GLN
1	A	430	ASN
1	A	445	GLN
1	A	478	GLN
1	A	516	ASN
1	A	543	ASN
1	A	566	ASN
1	A	584	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	587/610 (96%)	-0.26	15 (2%) 57 62	19, 32, 58, 81	22 (3%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	6.1
1	A	211	VAL	4.6
1	A	58	GLY	4.2
1	A	209	GLY	3.5
1	A	66	ALA	3.2
1	A	225	SER	3.1
1	A	2	ALA	3.0
1	A	226	LYS	2.9
1	A	604	PHE	2.7
1	A	67	PHE	2.7
1	A	602	VAL	2.5
1	A	601	GLU	2.4
1	A	210	ASN	2.2
1	A	205	GLU	2.2
1	A	222	SER	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	BR	A	614	1/1	0.98	0.07	54,54,54,54	0
2	BR	A	616	1/1	0.98	0.10	53,53,53,53	1
2	BR	A	607	1/1	0.99	0.07	40,40,40,40	0
2	BR	A	608	1/1	0.99	0.06	55,55,55,55	0
2	BR	A	609	1/1	0.99	0.09	51,51,51,51	0
2	BR	A	610	1/1	0.99	0.05	47,47,47,47	0
2	BR	A	611	1/1	0.99	0.10	39,39,39,39	1
2	BR	A	612	1/1	0.99	0.06	57,57,57,57	0
2	BR	A	613	1/1	0.99	0.06	69,69,69,69	0
2	BR	A	605	1/1	0.99	0.08	44,44,44,44	0
2	BR	A	615	1/1	0.99	0.07	54,54,54,54	0
2	BR	A	606	1/1	0.99	0.09	36,36,36,36	0
2	BR	A	617	1/1	0.99	0.18	51,51,51,51	1

6.5 Other polymers [i](#)

There are no such residues in this entry.