



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:17 PM EDT

PDB ID : 5LHC  
Title : The structure of D456A mutant of Nt.BspD6I nicking endonuclease at 0.24 nm resolution .  
Authors : Kachalova, G.S.; Yunusova, A.K.; Popov, A.N.; Artyukh, R.I.; Perevyazova, T.A.; Bartunik, H.D.; Zheleznaya, L.A.  
Deposited on : 2016-07-10  
Resolution : 2.40 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](mailto: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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

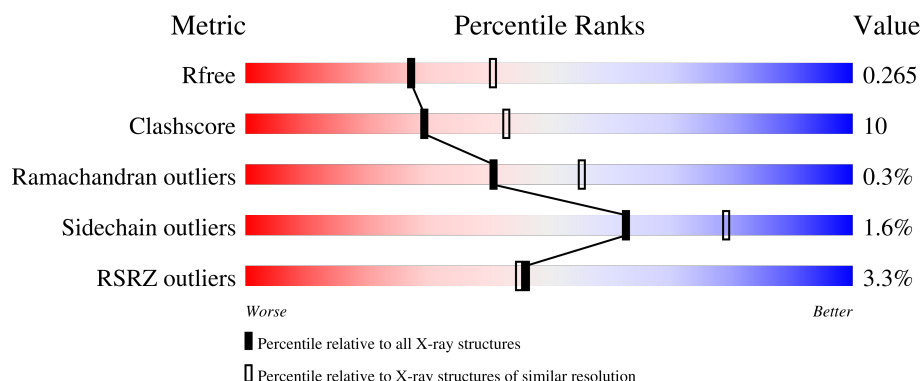
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	 4% 74% 20% • 5%
1	B	610	 2% 80% 15% • 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
3	PO4	A	703	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9854 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	579	Total	C	N	O	S	0	0	0
			4806	3092	811	888	15			
1	B	582	Total	C	N	O	S	0	1	0
			4831	3110	815	891	15			

There are 14 discrepancies between the modelled and reference sequences:

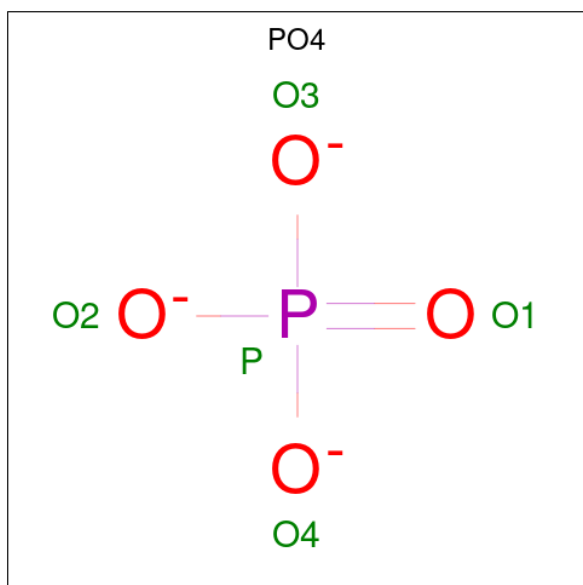
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q8GCA3
A	-4	HIS	-	expression tag	UNP Q8GCA3
A	-3	HIS	-	expression tag	UNP Q8GCA3
A	-2	HIS	-	expression tag	UNP Q8GCA3
A	-1	HIS	-	expression tag	UNP Q8GCA3
A	0	HIS	-	expression tag	UNP Q8GCA3
A	456	ALA	ASP	engineered mutation	UNP Q8GCA3
B	-5	HIS	-	expression tag	UNP Q8GCA3
B	-4	HIS	-	expression tag	UNP Q8GCA3
B	-3	HIS	-	expression tag	UNP Q8GCA3
B	-2	HIS	-	expression tag	UNP Q8GCA3
B	-1	HIS	-	expression tag	UNP Q8GCA3
B	0	HIS	-	expression tag	UNP Q8GCA3
B	456	ALA	ASP	engineered mutation	UNP Q8GCA3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

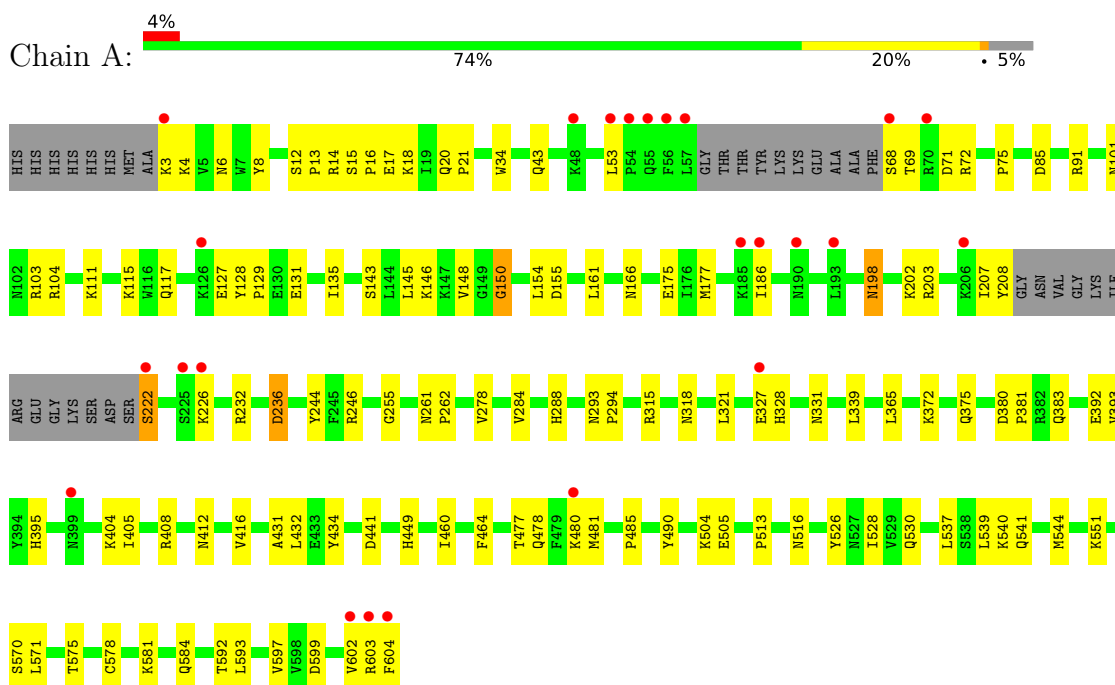
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	118	Total O 118 118	0	0

### 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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.35Å 92.67Å 113.97Å 90.00° 105.75° 90.00°	Depositor
Resolution (Å)	19.00 – 2.40 18.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.00-2.40) 99.2 (18.99-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.195 , 0.265 0.195 , 0.265	Depositor DCC
$R_{free}$ test set	2968 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4261e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, GOL

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	0.74	0/4902	0.87	5/6598 (0.1%)
1	B	0.78	0/4931	0.89	7/6635 (0.1%)
All	All	0.76	0/9833	0.88	12/13233 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	203	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	B	533	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	B	316	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	53	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	321	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	A	150	GLY	N-CA-C	-5.56	99.20	113.10
1	A	91	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	246	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	441	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	321	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	568	MET	CG-SD-CE	5.17	108.48	100.20

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	4806	0	4857	107	0
1	B	4831	0	4883	80	1
2	A	6	0	8	1	0
2	B	18	0	24	5	0
3	A	10	0	0	6	0
3	B	10	0	0	1	0
4	A	55	0	0	4	0
4	B	118	0	0	6	0
All	All	9854	0	9772	185	1

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 10.

All (185) 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:392:GLU:OE2	1:A:395:HIS:HD2	1.20	1.19
1:B:175:GLU:OE2	1:B:203:ARG:NH1	1.80	1.14
1:A:339:LEU:HG	1:A:365:LEU:CD2	1.81	1.10
1:A:392:GLU:OE2	1:A:395:HIS:CD2	2.06	1.08
2:B:703:GOL:H31	4:B:861:HOH:O	1.54	1.07
1:B:339:LEU:HG	1:B:365:LEU:CD2	1.88	1.01
1:B:331:ASN:HD21	1:B:375:GLN:HE22	0.99	0.99
1:A:3:LYS:HD3	1:A:129:PRO:HG3	1.47	0.97
1:A:331:ASN:HD21	1:A:375:GLN:HE22	1.13	0.94
1:B:339:LEU:HG	1:B:365:LEU:HD21	1.47	0.94
1:A:339:LEU:HG	1:A:365:LEU:HD21	1.49	0.92
1:A:175:GLU:OE2	1:A:203:ARG:NH1	2.04	0.91
1:A:339:LEU:CD2	1:A:365:LEU:HD23	2.07	0.85
1:B:383:GLN:NE2	2:B:702:GOL:O1	2.11	0.83
1:B:377:ASP:HB3	1:B:383:GLN:HE22	1.43	0.83
1:B:175:GLU:CD	1:B:203:ARG:HH12	1.83	0.82
1:A:3:LYS:HD3	1:A:129:PRO:CG	2.10	0.82
1:A:117:GLN:HE22	1:A:278:VAL:H	1.26	0.82
1:A:449:HIS:CD2	3:A:703:PO4:O3	2.33	0.81
1:B:117:GLN:HE22	1:B:278:VAL:H	1.27	0.80
1:B:477:THR:HG22	4:B:878:HOH:O	1.82	0.79
1:B:339:LEU:CD2	1:B:365:LEU:HD23	2.13	0.78
1:B:339:LEU:HD21	1:B:365:LEU:HD23	1.65	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:HG3	1:A:18:LYS:HB2	1.66	0.78
1:A:339:LEU:CG	1:A:365:LEU:CD2	2.62	0.77
1:A:198:ASN:HD21	1:A:202:LYS:HE3	1.50	0.77
1:B:321:LEU:CD1	1:B:369:LEU:HB3	2.15	0.77
1:A:14:ARG:NH2	1:A:236:ASP:CG	2.39	0.76
1:A:327:GLU:HG2	1:A:328:HIS:N	2.02	0.75
1:B:339:LEU:CG	1:B:365:LEU:CD2	2.64	0.74
1:B:331:ASN:ND2	1:B:375:GLN:HE22	1.83	0.72
1:A:412:ASN:ND2	3:A:703:PO4:O4	2.22	0.72
1:A:14:ARG:HH22	1:A:236:ASP:CG	1.93	0.72
1:B:331:ASN:HD21	1:B:375:GLN:NE2	1.83	0.71
1:B:377:ASP:HB3	1:B:383:GLN:NE2	2.05	0.71
1:B:177:MET:HE2	1:B:177:MET:HA	1.74	0.70
1:A:392:GLU:CD	1:A:395:HIS:HD2	1.93	0.69
1:B:339:LEU:CD2	1:B:365:LEU:CD2	2.70	0.69
1:A:339:LEU:HG	1:A:365:LEU:HD23	1.71	0.69
1:A:20:GLN:HB3	1:A:21:PRO:HD3	1.76	0.68
1:B:177:MET:HA	1:B:177:MET:CE	2.24	0.68
1:A:339:LEU:HD21	1:A:365:LEU:HD23	1.74	0.68
1:A:480:LYS:CE	1:B:178:GLN:HE21	2.07	0.68
1:B:321:LEU:HD11	1:B:369:LEU:HB3	1.74	0.68
1:A:72:ARG:O	1:A:75:PRO:HD2	1.95	0.67
1:A:339:LEU:CG	1:A:365:LEU:HD23	2.25	0.66
1:B:104:ARG:NH2	3:B:704:PO4:O4	2.26	0.66
1:A:480:LYS:NZ	1:B:178:GLN:HE21	1.94	0.65
1:B:20:GLN:HB3	1:B:21:PRO:HD3	1.79	0.65
1:B:364:GLU:HG2	4:B:865:HOH:O	1.97	0.64
1:A:101:ASN:HD22	1:A:103:ARG:HH12	1.46	0.64
1:A:103:ARG:HD2	4:A:824:HOH:O	1.97	0.64
1:B:177:MET:HE1	1:B:180:ARG:HH11	1.64	0.63
1:B:581:LYS:HB2	1:B:584:GLN:HG2	1.80	0.62
1:A:6:ASN:HA	1:A:161:LEU:O	2.00	0.62
1:A:14:ARG:NH2	1:A:236:ASP:OD2	2.33	0.62
1:A:513:PRO:HA	1:A:539:LEU:HB3	1.82	0.61
1:A:603:ARG:O	1:A:604:PHE:HB2	2.01	0.60
1:B:69:THR:O	1:B:71:ASP:N	2.34	0.60
1:B:478:GLN:HE22	1:B:516:ASN:H	1.47	0.60
1:A:327:GLU:HG2	1:A:328:HIS:H	1.67	0.60
1:A:3:LYS:HD3	1:A:129:PRO:CD	2.32	0.59
1:A:4:LYS:HD3	1:A:127:GLU:OE2	2.02	0.59
1:B:363:LYS:CB	2:B:703:GOL:H32	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLN:HG3	1:B:102:ASN:HD22	1.67	0.59
1:A:339:LEU:CD2	1:A:365:LEU:CD2	2.80	0.59
1:B:177:MET:HE2	1:B:180:ARG:HD2	1.83	0.59
1:B:158:MET:HG2	1:B:200:PHE:CD1	2.38	0.58
1:A:449:HIS:HD2	3:A:703:PO4:O1	1.85	0.58
1:B:201:PHE:CE2	1:B:205:GLU:OE1	2.56	0.58
1:B:363:LYS:HB3	2:B:703:GOL:H32	1.86	0.58
1:A:505:GLU:HG3	4:A:803:HOH:O	2.03	0.57
1:A:551:LYS:HD2	1:A:602:VAL:HG11	1.86	0.57
1:A:101:ASN:HD22	1:A:103:ARG:NH1	2.01	0.57
1:A:412:ASN:O	1:A:416:VAL:HG23	2.04	0.57
1:A:490:TYR:C	1:A:490:TYR:CD1	2.77	0.57
1:A:203:ARG:HG3	1:A:203:ARG:HH11	1.69	0.57
1:A:207:ILE:HG22	1:A:208:TYR:CD1	2.39	0.57
1:A:177:MET:HA	1:A:177:MET:CE	2.35	0.56
1:A:480:LYS:HE3	1:B:178:GLN:HE21	1.70	0.56
1:B:69:THR:O	1:B:72:ARG:N	2.38	0.56
1:B:177:MET:HE1	1:B:180:ARG:NH1	2.20	0.56
1:B:333:LYS:HB3	4:B:818:HOH:O	2.06	0.55
1:B:478:GLN:NE2	1:B:516:ASN:H	2.05	0.55
1:A:16:PRO:HG3	1:A:244:TYR:HA	1.89	0.55
1:B:222:SER:N	1:B:226:LYS:HZ3	2.04	0.55
1:A:449:HIS:HD2	3:A:703:PO4:P	2.31	0.54
1:A:478:GLN:NE2	1:A:516:ASN:HB3	2.23	0.54
1:A:551:LYS:CD	1:A:602:VAL:HG11	2.37	0.54
1:A:526:TYR:CD2	1:A:530:GLN:HG3	2.43	0.54
1:A:481:MET:O	1:A:485:PRO:HG2	2.08	0.53
1:A:155:ASP:OD1	2:A:701:GOL:H11	2.08	0.53
1:B:516:ASN:HD22	1:B:519:THR:H	1.57	0.53
1:A:593:LEU:O	1:A:597:VAL:HG23	2.09	0.53
1:A:541:GLN:HG2	1:A:593:LEU:HD22	1.90	0.53
1:A:115:LYS:NZ	1:A:293:ASN:O	2.42	0.53
1:B:526:TYR:CD2	1:B:530:GLN:HG3	2.45	0.51
1:B:39:GLY:O	1:B:43:GLN:HG3	2.10	0.51
1:A:198:ASN:ND2	1:A:202:LYS:HE3	2.21	0.51
1:A:203:ARG:NH1	1:A:203:ARG:HG3	2.26	0.51
1:B:284:VAL:O	1:B:288:HIS:HD2	1.94	0.51
1:A:431:ALA:HB3	1:A:434:TYR:CZ	2.46	0.51
1:A:478:GLN:HE22	1:A:516:ASN:H	1.57	0.51
1:A:327:GLU:CG	1:A:328:HIS:N	2.73	0.50
1:A:477:THR:O	1:A:480:LYS:HB3	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:LEU:HD11	1:B:369:LEU:CB	2.40	0.50
1:B:321:LEU:HD13	1:B:369:LEU:HB3	1.92	0.50
1:A:85:ASP:HB2	4:A:835:HOH:O	2.11	0.50
1:A:541:GLN:HG2	1:A:593:LEU:CD2	2.41	0.50
1:A:13:PRO:CG	1:A:18:LYS:HB2	2.39	0.49
1:A:143:SER:O	1:A:146:LYS:HB2	2.12	0.49
1:A:372:LYS:O	1:A:375:GLN:HB2	2.12	0.49
1:A:404:LYS:O	1:A:408:ARG:NH1	2.46	0.49
1:A:207:ILE:HG22	1:A:208:TYR:CE1	2.47	0.49
1:A:34:TRP:O	1:A:43:GLN:NE2	2.46	0.48
1:B:177:MET:CE	1:B:180:ARG:HD2	2.43	0.48
1:A:4:LYS:HG3	1:A:128:TYR:CZ	2.49	0.48
1:A:449:HIS:CD2	3:A:703:PO4:P	3.06	0.47
1:B:45:ALA:HA	1:B:48:LYS:HE2	1.97	0.47
1:B:339:LEU:CG	1:B:365:LEU:HD23	2.41	0.47
1:A:177:MET:HA	1:A:177:MET:HE2	1.95	0.47
1:B:392:GLU:OE1	1:B:395:HIS:ND1	2.44	0.47
1:B:34:TRP:O	1:B:43:GLN:NE2	2.47	0.47
1:B:35:LYS:HB3	1:B:35:LYS:HE2	1.58	0.47
1:A:540:LYS:HG2	1:A:544:MET:HE3	1.97	0.47
1:B:44:GLU:HA	1:B:44:GLU:OE1	2.15	0.47
1:B:4:LYS:HG3	1:B:128:TYR:CZ	2.50	0.46
1:A:3:LYS:CD	1:A:129:PRO:CG	2.88	0.46
1:B:429:GLY:O	1:B:430:ASN:HB2	2.16	0.46
1:A:68:SER:OG	1:A:71:ASP:OD2	2.33	0.46
1:B:3:LYS:HD2	1:B:132:GLU:OE1	2.16	0.46
1:B:371:LYS:NZ	2:B:701:GOL:H31	2.31	0.46
1:B:443:GLU:O	1:B:444:LEU:HB2	2.14	0.46
1:B:490:TYR:CD1	1:B:490:TYR:C	2.89	0.46
1:A:175:GLU:O	1:A:175:GLU:HG2	2.16	0.46
1:A:255:GLY:HA2	1:A:408:ARG:O	2.16	0.46
1:B:69:THR:O	1:B:70:ARG:C	2.53	0.46
1:B:69:THR:C	1:B:71:ASP:N	2.68	0.46
1:A:12:SER:HA	1:A:13:PRO:HA	1.72	0.45
1:A:3:LYS:CD	1:A:129:PRO:CD	2.95	0.45
1:B:117:GLN:NE2	1:B:277:VAL:HA	2.32	0.45
1:B:480:LYS:NZ	1:B:481:MET:HG3	2.32	0.45
1:B:551:LYS:HE3	1:B:604:PHE:CD1	2.51	0.45
1:A:537:LEU:HD22	1:A:541:GLN:HB3	1.98	0.45
1:A:318:ASN:HD22	1:A:339:LEU:HD21	1.82	0.45
1:A:232:ARG:HH11	1:A:232:ARG:HB2	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:SER:HB3	1:A:592:THR:CG2	2.47	0.44
1:A:380:ASP:HA	1:A:381:PRO:HD2	1.68	0.44
1:A:3:LYS:CD	1:A:129:PRO:HG3	2.34	0.44
1:A:513:PRO:HA	1:A:539:LEU:CB	2.45	0.44
1:A:222:SER:O	1:A:226:LYS:HG3	2.17	0.44
1:A:581:LYS:HB3	1:A:584:GLN:HG2	2.00	0.44
1:B:245:PHE:HB3	1:B:251:PHE:CD1	2.52	0.44
1:A:175:GLU:CD	1:A:203:ARG:HH12	2.12	0.44
1:B:431:ALA:HB3	1:B:434:TYR:CZ	2.53	0.43
1:A:327:GLU:CG	1:A:328:HIS:H	2.29	0.43
1:B:551:LYS:HE3	1:B:604:PHE:CE1	2.53	0.43
1:B:531:ASN:HA	4:B:836:HOH:O	2.19	0.43
1:A:261:ASN:HA	1:A:262:PRO:HD2	1.66	0.43
1:B:367:LEU:HD12	1:B:367:LEU:HA	1.86	0.43
1:A:571:LEU:O	1:A:575:THR:HG23	2.19	0.43
1:A:135:ILE:HG13	1:A:166:ASN:OD1	2.18	0.43
1:A:284:VAL:O	1:A:288:HIS:HD2	2.02	0.43
1:A:464:PHE:HA	1:A:504:LYS:HB3	2.01	0.43
1:A:145:LEU:CD2	1:A:150:GLY:HA2	2.49	0.42
1:A:15:SER:HB2	1:A:17:GLU:OE1	2.19	0.42
1:B:74:ALA:N	1:B:75:PRO:CD	2.81	0.42
1:A:581:LYS:O	1:A:584:GLN:N	2.51	0.42
1:B:12:SER:HA	1:B:13:PRO:HA	1.85	0.42
1:B:20:GLN:HG3	1:B:102:ASN:ND2	2.32	0.42
1:B:299:PHE:HB2	1:B:302:GLU:HG3	2.01	0.42
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.85	0.41
1:A:43:GLN:HB3	1:A:69:THR:HG21	2.03	0.41
1:A:104:ARG:NH2	3:A:702:PO4:O1	2.43	0.41
1:A:432:LEU:N	1:A:460:ILE:O	2.51	0.41
1:A:288:HIS:HE1	4:A:809:HOH:O	2.03	0.41
1:B:101:ASN:HD22	1:B:103:ARG:HH12	1.67	0.41
1:A:405:ILE:O	1:A:408:ARG:N	2.47	0.41
1:B:16:PRO:HG3	1:B:247:TYR:HB2	2.02	0.41
1:A:111:LYS:HD2	1:A:294:PRO:O	2.20	0.41
1:A:135:ILE:HA	1:A:166:ASN:OD1	2.21	0.41
1:B:176:ILE:HG22	1:B:177:MET:HE3	2.03	0.41
1:B:270:GLU:OE2	1:B:300:SER:N	2.36	0.40
1:B:366:GLN:HE21	1:B:370:LYS:NZ	2.19	0.40
1:B:494:LYS:HD2	4:B:838:HOH:O	2.21	0.40

All (1) 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:B:315:ARG:NH1	1:B:529:VAL:O[2_556]	2.16	0.04

## 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	573/610 (94%)	537 (94%)	33 (6%)	3 (0%)	29	41
1	B	577/610 (95%)	551 (96%)	25 (4%)	1 (0%)	47	62
All	All	1150/1220 (94%)	1088 (95%)	58 (5%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	ARG
1	A	393	VAL
1	A	186	ILE
1	A	148	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	529/553 (96%)	517 (98%)	12 (2%)	50	70
1	B	531/553 (96%)	526 (99%)	5 (1%)	78	90
All	All	1060/1106 (96%)	1043 (98%)	17 (2%)	62	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	TYR
1	A	131	GLU
1	A	154	LEU
1	A	198	ASN
1	A	222	SER
1	A	236	ASP
1	A	315	ARG
1	A	321	LEU
1	A	383	GLN
1	A	528	ILE
1	A	578	CYS
1	A	599	ASP
1	B	8	TYR
1	B	69	THR
1	B	230	LYS
1	B	257	GLN
1	B	480	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	117	GLN
1	A	178	GLN
1	A	181	ASN
1	A	198	ASN
1	A	257	GLN
1	A	280	ASN
1	A	288	HIS
1	A	344	ASN
1	A	366	GLN
1	A	375	GLN
1	A	395	HIS
1	A	449	HIS
1	A	478	GLN
1	A	516	ASN
1	B	101	ASN
1	B	102	ASN
1	B	117	GLN
1	B	136	ASN
1	B	178	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	181	ASN
1	B	198	ASN
1	B	280	ASN
1	B	288	HIS
1	B	344	ASN
1	B	366	GLN
1	B	375	GLN
1	B	383	GLN
1	B	478	GLN
1	B	516	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	B	704	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	A	702	-	4,4,4	0.93	0	6,6,6	0.43	0
2	GOL	B	702	-	5,5,5	0.35	0	5,5,5	1.09	0
3	PO4	A	703	-	4,4,4	0.91	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	B	705	-	4,4,4	0.92	0	6,6,6	0.43	0
2	GOL	A	701	-	5,5,5	0.25	0	5,5,5	0.28	0
2	GOL	B	703	-	5,5,5	0.26	0	5,5,5	0.28	0
2	GOL	B	701	-	5,5,5	0.26	0	5,5,5	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	702	-	-	2/4/4/4	-
2	GOL	A	701	-	-	4/4/4/4	-
2	GOL	B	703	-	-	1/4/4/4	-
2	GOL	B	701	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GOL	O1-C1-C2-C3
2	B	701	GOL	C1-C2-C3-O3
2	A	701	GOL	C1-C2-C3-O3
2	B	702	GOL	O1-C1-C2-C3
2	A	701	GOL	O1-C1-C2-O2
2	B	701	GOL	O2-C2-C3-O3
2	B	702	GOL	O1-C1-C2-O2
2	B	703	GOL	O1-C1-C2-C3
2	A	701	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	PO4	1	0
3	A	702	PO4	1	0
2	B	702	GOL	1	0
3	A	703	PO4	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GOL	1	0
2	B	703	GOL	3	0
2	B	701	GOL	1	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	579/610 (94%)	-0.02	24 (4%) 37 36	34, 62, 104, 157	0
1	B	582/610 (95%)	-0.22	14 (2%) 59 57	30, 51, 97, 158	0
All	All	1161/1220 (95%)	-0.12	38 (3%) 46 45	30, 57, 101, 158	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	PHE	9.0
1	B	57	LEU	8.3
1	A	603	ARG	6.1
1	A	604	PHE	6.0
1	B	58	GLY	5.5
1	B	66	ALA	5.4
1	A	57	LEU	4.9
1	B	603	ARG	4.6
1	A	56	PHE	4.5
1	A	185	LYS	4.5
1	A	226	LYS	3.9
1	B	68	SER	3.7
1	A	53	LEU	3.7
1	A	602	VAL	3.6
1	B	604	PHE	3.4
1	B	56	PHE	3.4
1	A	193	LEU	3.1
1	B	602	VAL	3.0
1	B	53	LEU	3.0
1	A	190	ASN	3.0
1	A	222	SER	2.9
1	A	225	SER	2.9
1	A	480	LYS	2.9
1	A	186	ILE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	55	GLN	2.5
1	A	3	LYS	2.5
1	A	68	SER	2.5
1	A	70	ARG	2.4
1	A	54	PRO	2.4
1	A	327	GLU	2.3
1	B	48	LYS	2.3
1	A	206	LYS	2.2
1	B	224	LYS	2.2
1	B	185	LYS	2.2
1	A	48	LYS	2.1
1	B	37	VAL	2.1
1	A	399	ASN	2.1
1	A	126	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	B	702	6/6	0.81	0.33	30,38,44,46	6
3	PO4	A	702	5/5	0.82	0.40	44,49,55,61	5
2	GOL	A	701	6/6	0.84	0.28	37,42,44,44	6
2	GOL	B	703	6/6	0.88	0.43	43,48,51,53	6
3	PO4	A	703	5/5	0.88	0.20	42,49,52,52	5
3	PO4	B	704	5/5	0.90	0.42	41,47,57,65	5
3	PO4	B	705	5/5	0.92	0.18	46,47,50,53	5
2	GOL	B	701	6/6	0.93	0.17	29,32,36,37	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.