



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FOK
Title : STRUCTURE OF RESTRICTION ENDONUCLEASE FOKI BOUND TO DNA
Authors : Aggarwal, D.A.; Wah, J.A.; Hirsch, L.F.; Dorner, I.; Schildkraut, A.K.
Deposited on : 1997-04-18
Resolution : 2.80 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

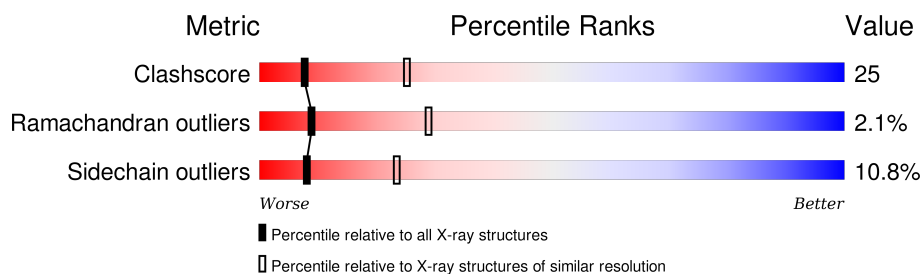
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	20	
2	C	20	
3	A	576	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5527 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 DNA chain called DNA (5'-D(*TP*CP*GP*GP*AP*TP*GP*AP*TP*AP*AP*CP*GP*CP*TP*AP*G P*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	20	Total	C	N	O	P	0	0	0
			409	196	77	117	19			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*GP*AP*CP*TP*AP*GP*CP*GP*TP*TP*AP*TP*CP*AP*T P*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			405	195	72	119	19			

- Molecule 3 is a protein called PROTEIN (FOKI RESTRICTION ENDONUCLEASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	568	Total	C	N	O	S	0	0	0
			4541	2908	780	842	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		
4	B	15	Total	O	0	0
			15	15		
4	C	22	Total	O	0	0
			22	22		

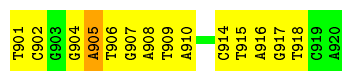
3 Residue-property plots

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.

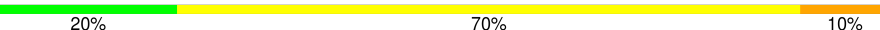
Note EDS was not executed.

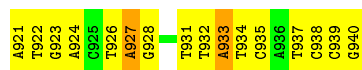
- Molecule 1: DNA (5'-D(*TP*CP*GP*GP*AP*TP*GP*AP*TP*AP*AP*CP*GP*CP*TP*AP*G P*TP*CP*A)-3')

Chain B: 



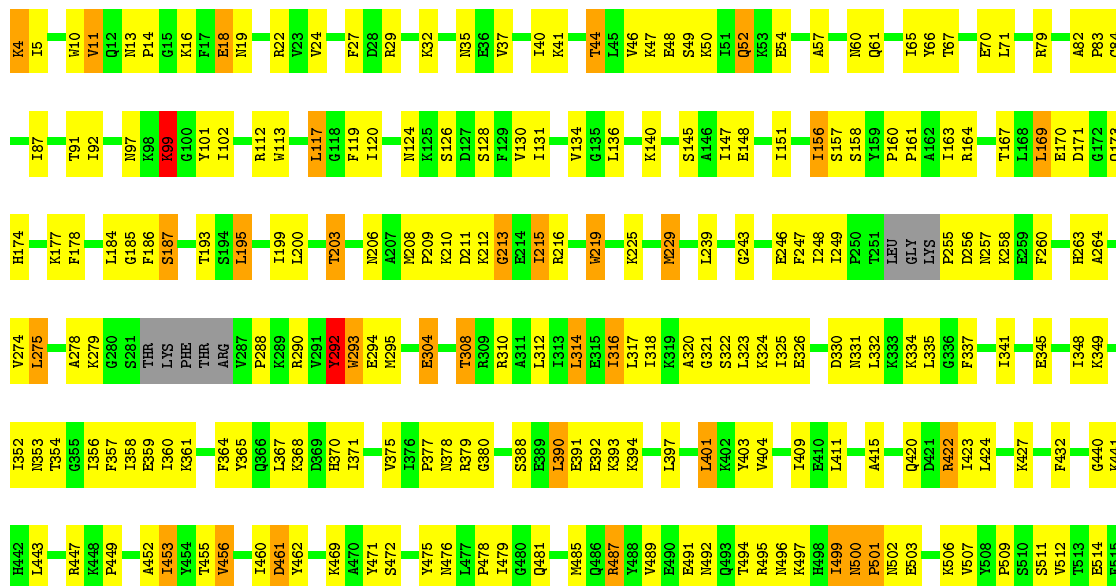
- Molecule 2: DNA (5'-D(*AP*TP*GP*AP*CP*TP*AP*GP*CP*GP*TP*TP*AP*TP*CP*AP*T P*CP*CP*G)-3')

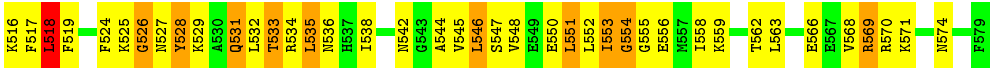
Chain C: 



- Molecule 3: PROTEIN (FOKI RESTRICTION ENDONUCLEASE)

Chain A: 





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.59 Å 119.34 Å 71.52 Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.9 (8.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.214 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5527	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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	B	0.74	0/459	0.85	0/707
2	C	0.71	0/453	0.94	0/697
3	A	0.56	2/4626 (0.0%)	0.82	7/6227 (0.1%)
All	All	0.59	2/5538 (0.0%)	0.84	7/7631 (0.1%)

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	B	0	1
2	C	0	3
3	A	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	18	GLU	CG-CD	5.74	1.60	1.51
3	A	18	GLU	CB-CG	5.60	1.62	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	518	LEU	CA-CB-CG	7.33	132.16	115.30
3	A	526	GLY	N-CA-C	6.58	129.55	113.10
3	A	499	ILE	N-CA-C	-6.58	93.24	111.00
3	A	99	LYS	N-CA-C	-6.38	93.78	111.00
3	A	255	PRO	N-CA-CB	6.20	110.74	103.30
3	A	213	GLY	N-CA-C	-6.11	97.83	113.10
3	A	554	GLY	N-CA-C	-5.29	99.89	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	292	TYR	Sidechain
1	B	905	DA	Sidechain
2	C	927	DA	Sidechain
2	C	931	DT	Sidechain
2	C	933	DA	Sidechain

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	B	409	0	227	14	0
2	C	405	0	228	20	0
3	A	4541	0	4606	229	0
4	A	135	0	0	24	0
4	B	15	0	0	0	0
4	C	22	0	0	5	0
All	All	5527	0	5061	261	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 25.

All (261) 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)
2:C:932:DT:H1'	4:C:754:HOH:O	1.52	1.09
2:C:921:DA:H2''	2:C:922:DT:OP2	1.71	0.88
3:A:318:ILE:HD11	3:A:371:ILE:HD11	1.59	0.83
3:A:516:LYS:HE2	4:A:651:HOH:O	1.79	0.82
3:A:422:ARG:HB3	4:A:744:HOH:O	1.80	0.82
3:A:360:ILE:HG12	3:A:365:TYR:HD1	1.48	0.78
2:C:934:DT:H2''	2:C:935:DC:O5'	1.84	0.77
3:A:478:PRO:HB2	3:A:481:GLN:HG2	1.65	0.77
3:A:341:ILE:HB	4:A:650:HOH:O	1.84	0.77
3:A:348:ILE:O	3:A:352:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:359:GLU:HG3	3:A:368:LYS:HG3	1.68	0.76
1:B:904:DG:O6	3:A:225:LYS:HE2	1.85	0.76
3:A:160:PRO:HB2	3:A:161:PRO:HD3	1.68	0.75
3:A:209:PRO:HA	3:A:212:LYS:HG2	1.68	0.74
1:B:915:DT:H2''	1:B:916:DA:C8	2.22	0.74
2:C:927:DA:H2''	2:C:928:DG:H5'	1.70	0.73
3:A:469:LYS:HE3	3:A:471:TYR:HD1	1.53	0.72
3:A:275:LEU:O	3:A:279:LYS:HB2	1.90	0.72
3:A:332:LEU:HD22	3:A:337:PHE:HB2	1.72	0.70
2:C:926:DT:H2''	2:C:927:DA:N7	2.06	0.70
3:A:359:GLU:CG	3:A:368:LYS:HG3	2.22	0.70
3:A:324:LYS:HG3	3:A:364:PHE:CE2	2.26	0.70
3:A:210:LYS:H	3:A:210:LYS:HD2	1.56	0.69
3:A:22:ARG:NH1	3:A:91:THR:HG22	2.07	0.69
3:A:536:ASN:OD1	3:A:542:ASN:HA	1.92	0.69
3:A:568:VAL:O	3:A:571:LYS:HB2	1.93	0.69
3:A:415:ALA:HA	3:A:424:LEU:HD22	1.74	0.69
3:A:409:ILE:HG12	4:A:747:HOH:O	1.92	0.69
3:A:83:PRO:HD2	4:A:680:HOH:O	1.93	0.68
3:A:569:ARG:HD2	3:A:570:ARG:HG2	1.76	0.68
3:A:469:LYS:HE3	3:A:471:TYR:CD1	2.28	0.68
3:A:167:THR:O	3:A:170:GLU:HG3	1.93	0.68
3:A:360:ILE:HG12	3:A:365:TYR:CD1	2.29	0.67
3:A:411:LEU:HD21	3:A:427:LYS:HB3	1.77	0.67
1:B:917:DG:H2''	1:B:918:DT:OP2	1.96	0.66
3:A:11:VAL:HG11	3:A:113:TRP:HB2	1.78	0.66
3:A:569:ARG:HH11	3:A:569:ARG:HB2	1.60	0.65
3:A:249:ILE:O	3:A:257:ASN:HB3	1.96	0.64
3:A:331:ASN:HA	3:A:334:LYS:NZ	2.12	0.63
3:A:485:MET:CE	3:A:517:PHE:HB2	2.29	0.63
3:A:485:MET:O	3:A:489:VAL:HG23	1.98	0.63
3:A:492:ASN:HD21	3:A:495:ARG:NH2	1.97	0.63
3:A:316:ILE:HD11	3:A:335:LEU:CD1	2.28	0.63
3:A:500:ASN:HD21	3:A:502:ASN:ND2	1.96	0.63
3:A:479:ILE:HG12	3:A:531:GLN:NE2	2.13	0.62
3:A:485:MET:HE1	3:A:517:PHE:HB2	1.81	0.62
3:A:312:LEU:O	3:A:316:ILE:HD13	2.00	0.61
3:A:323:LEU:HD12	3:A:323:LEU:N	2.15	0.61
2:C:927:DA:H2''	2:C:928:DG:C5'	2.31	0.61
3:A:248:ILE:HA	3:A:257:ASN:O	2.01	0.61
3:A:292:TYR:O	3:A:295:MET:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:569:ARG:HD2	3:A:570:ARG:CG	2.32	0.60
3:A:397:LEU:HB3	4:A:747:HOH:O	2.01	0.59
3:A:314:LEU:HD11	3:A:356:ILE:HD13	1.83	0.59
3:A:304:GLU:O	3:A:308:THR:HG22	2.03	0.59
2:C:937:DT:H2''	2:C:938:DC:C5'	2.32	0.59
1:B:901:DT:H6	1:B:901:DT:HO5'	1.48	0.59
3:A:460:ILE:HG23	3:A:460:ILE:O	2.02	0.59
3:A:212:LYS:HA	3:A:215:ILE:HG12	1.84	0.58
3:A:566:GLU:O	3:A:569:ARG:HG3	2.03	0.58
1:B:904:DG:H2''	1:B:905:DA:O5'	2.04	0.57
3:A:325:ILE:HG12	3:A:365:TYR:CE2	2.40	0.57
3:A:317:LEU:HD13	3:A:358:ILE:HD13	1.86	0.57
1:B:909:DT:H2''	1:B:910:DA:C8	2.39	0.57
3:A:357:PHE:O	3:A:367:LEU:HD12	2.05	0.57
3:A:487:ARG:HB2	3:A:487:ARG:HH11	1.68	0.57
3:A:156:ILE:HG22	3:A:157:SER:N	2.19	0.57
2:C:921:DA:C2'	2:C:922:DT:OP2	2.50	0.56
3:A:316:ILE:HD11	3:A:335:LEU:HD11	1.87	0.56
3:A:4:LYS:HE2	3:A:4:LYS:HA	1.87	0.56
3:A:499:ILE:HB	4:A:759:HOH:O	2.05	0.56
2:C:932:DT:H73	4:C:726:HOH:O	2.05	0.55
3:A:469:LYS:CE	3:A:471:TYR:HD1	2.20	0.55
3:A:32:LYS:O	3:A:35:ASN:HB3	2.05	0.55
3:A:528:TYR:HB2	3:A:545:VAL:HG21	1.87	0.55
3:A:117:LEU:N	3:A:117:LEU:HD23	2.21	0.55
3:A:46:VAL:O	3:A:52:GLN:HG3	2.05	0.55
3:A:124:ASN:H	3:A:124:ASN:HD22	1.54	0.55
3:A:19:ASN:ND2	3:A:92:ILE:HG23	2.22	0.54
3:A:452:ALA:CB	3:A:507:VAL:HG11	2.37	0.54
3:A:19:ASN:HB3	3:A:92:ILE:HD12	1.90	0.54
3:A:239:LEU:HD22	3:A:274:VAL:HG21	1.90	0.54
3:A:390:LEU:CD1	3:A:394:LYS:HD2	2.38	0.54
2:C:934:DT:C2'	2:C:935:DC:O5'	2.56	0.54
3:A:491:GLU:OE2	3:A:500:ASN:HB2	2.07	0.54
3:A:199:ILE:O	3:A:203:THR:HG23	2.07	0.54
2:C:933:DA:C5'	4:C:754:HOH:O	2.56	0.54
2:C:927:DA:H1'	2:C:928:DG:H5''	1.90	0.54
2:C:937:DT:H2''	2:C:938:DC:H5''	1.89	0.54
3:A:462:TYR:CE1	3:A:569:ARG:HB3	2.43	0.54
1:B:914:DC:C2'	1:B:915:DT:H72	2.38	0.54
3:A:542:ASN:CB	3:A:574:ASN:HD21	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:293:TRP:HZ3	3:A:308:THR:HG22	1.73	0.53
3:A:147:ILE:O	3:A:151:ILE:HG13	2.08	0.53
3:A:528:TYR:O	3:A:532:LEU:HB2	2.09	0.53
3:A:492:ASN:HD21	3:A:495:ARG:HH21	1.55	0.53
3:A:509:PRO:HD2	3:A:512:VAL:HG21	1.91	0.52
3:A:478:PRO:HG3	4:A:698:HOH:O	2.08	0.52
3:A:22:ARG:NH1	3:A:91:THR:O	2.43	0.52
3:A:65:ILE:HG12	3:A:130:VAL:CG1	2.39	0.52
3:A:479:ILE:HG23	3:A:534:ARG:HH12	1.74	0.52
3:A:447:ARG:NE	3:A:447:ARG:HA	2.24	0.52
3:A:210:LYS:N	3:A:210:LYS:HD2	2.23	0.52
3:A:318:ILE:HD11	3:A:371:ILE:CD1	2.35	0.52
3:A:558:ILE:CD1	3:A:563:LEU:HG	2.40	0.52
3:A:524:PHE:CD2	3:A:545:VAL:HG13	2.45	0.51
3:A:29:ARG:NH2	3:A:60:ASN:O	2.44	0.51
3:A:16:LYS:HG2	3:A:18:GLU:OE1	2.09	0.51
3:A:37:VAL:HA	3:A:41:LYS:HB2	1.91	0.51
3:A:164:ARG:HG2	3:A:353:ASN:O	2.10	0.50
3:A:546:LEU:HD22	3:A:547:SER:N	2.25	0.50
3:A:13:ASN:N	3:A:14:PRO:HD2	2.27	0.50
3:A:509:PRO:HD2	3:A:512:VAL:CG2	2.42	0.50
3:A:533:THR:HA	3:A:536:ASN:HD22	1.77	0.50
3:A:177:LYS:HD3	3:A:263:HIS:CB	2.42	0.50
3:A:158:SER:HB2	3:A:290:ARG:NH2	2.27	0.49
3:A:494:THR:O	3:A:494:THR:HG23	2.12	0.49
3:A:54:GLU:O	3:A:57:ALA:HB3	2.12	0.49
3:A:22:ARG:HH11	3:A:91:THR:HG22	1.78	0.49
2:C:933:DA:H5'	4:C:754:HOH:O	2.12	0.49
3:A:177:LYS:HD3	3:A:263:HIS:HB2	1.94	0.49
3:A:246:GLU:HB3	3:A:258:LYS:HD2	1.94	0.49
3:A:178:PHE:CE1	3:A:195:LEU:HB3	2.48	0.49
3:A:99:LYS:HB3	3:A:101:TYR:CE1	2.47	0.49
3:A:288:PRO:HB3	3:A:370:HIS:ND1	2.28	0.49
3:A:216:ARG:NH2	3:A:260:PHE:CE1	2.81	0.49
3:A:469:LYS:HD2	3:A:471:TYR:HD1	1.78	0.48
3:A:359:GLU:HB3	3:A:361:LYS:NZ	2.29	0.48
3:A:447:ARG:HH22	3:A:487:ARG:NE	2.11	0.48
3:A:70:GLU:O	3:A:87:ILE:HG13	2.13	0.48
3:A:145:SER:HB2	3:A:148:GLU:HB2	1.96	0.48
3:A:341:ILE:O	3:A:345:GLU:HG3	2.14	0.48
3:A:492:ASN:ND2	3:A:495:ARG:NH2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:569:ARG:NH1	4:A:651:HOH:O	2.47	0.48
3:A:469:LYS:CD	3:A:471:TYR:HD1	2.27	0.48
3:A:492:ASN:ND2	3:A:495:ARG:HH21	2.11	0.48
3:A:119:PHE:O	3:A:120:ILE:HD12	2.13	0.48
3:A:147:ILE:H	3:A:147:ILE:HD12	1.79	0.48
3:A:321:GLY:HA2	4:A:716:HOH:O	2.14	0.48
3:A:10:TRP:HA	4:A:725:HOH:O	2.14	0.48
3:A:225:LYS:NZ	3:A:229:MET:SD	2.84	0.47
3:A:288:PRO:HB3	3:A:370:HIS:CE1	2.49	0.47
3:A:14:PRO:HB2	3:A:113:TRP:CE3	2.49	0.47
1:B:901:DT:C2'	1:B:902:DC:C5	2.97	0.47
3:A:469:LYS:HD2	3:A:471:TYR:CD1	2.49	0.47
3:A:22:ARG:NH1	3:A:91:THR:CG2	2.75	0.47
3:A:293:TRP:CD2	3:A:377:PRO:HD2	2.49	0.47
3:A:391:GLU:HB3	4:A:743:HOH:O	2.15	0.47
3:A:248:ILE:HG12	3:A:258:LYS:HG2	1.97	0.47
3:A:443:LEU:O	3:A:449:PRO:O	2.32	0.47
3:A:27:PHE:HB3	3:A:131:ILE:HB	1.96	0.47
3:A:475:TYR:O	3:A:524:PHE:HA	2.15	0.47
3:A:528:TYR:O	3:A:532:LEU:HD22	2.14	0.47
3:A:432:PHE:CD2	3:A:453:ILE:HD11	2.50	0.47
3:A:529:LYS:HB3	4:A:738:HOH:O	2.14	0.47
3:A:415:ALA:HA	3:A:424:LEU:CD2	2.44	0.47
2:C:937:DT:H2''	2:C:938:DC:H5'	1.97	0.46
3:A:209:PRO:HA	3:A:212:LYS:CG	2.42	0.46
3:A:532:LEU:O	3:A:536:ASN:ND2	2.49	0.46
3:A:518:LEU:HD21	3:A:546:LEU:HB2	1.96	0.46
3:A:455:THR:HG22	3:A:456:VAL:N	2.30	0.46
3:A:455:THR:HG22	3:A:461:ASP:OD1	2.16	0.46
3:A:11:VAL:HG12	3:A:14:PRO:CG	2.46	0.46
3:A:67:THR:OG1	3:A:70:GLU:HG3	2.15	0.46
2:C:922:DT:H1'	2:C:923:DG:C8	2.51	0.45
3:A:186:PHE:CD1	3:A:186:PHE:N	2.84	0.45
3:A:460:ILE:HG21	3:A:569:ARG:HG2	1.98	0.45
3:A:349:LYS:HA	3:A:349:LYS:HD3	1.80	0.45
3:A:476:ASN:HB2	3:A:527:ASN:CG	2.37	0.45
3:A:156:ILE:HA	3:A:156:ILE:HD13	1.74	0.45
3:A:169:LEU:HB3	4:A:602:HOH:O	2.17	0.45
3:A:532:LEU:HD21	3:A:544:ALA:HA	1.99	0.45
3:A:552:LEU:HD13	4:A:747:HOH:O	2.16	0.45
3:A:293:TRP:NE1	3:A:377:PRO:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:124:ASN:H	3:A:124:ASN:ND2	2.15	0.45
3:A:558:ILE:HD12	3:A:563:LEU:HG	1.99	0.44
3:A:397:LEU:HD13	4:A:747:HOH:O	2.17	0.44
3:A:552:LEU:C	3:A:554:GLY:H	2.21	0.44
3:A:293:TRP:CD1	3:A:294:GLU:N	2.86	0.44
3:A:243:GLY:O	3:A:264:ALA:HB3	2.17	0.44
3:A:550:GLU:HA	3:A:553:ILE:HG12	2.00	0.44
3:A:40:ILE:O	3:A:44:THR:HG23	2.17	0.44
3:A:403:TYR:HB2	3:A:556:GLU:OE1	2.17	0.44
3:A:460:ILE:HG13	3:A:569:ARG:NH2	2.33	0.43
3:A:555:GLY:O	3:A:559:LYS:HG2	2.17	0.43
3:A:200:LEU:HD23	3:A:219:TRP:CD1	2.53	0.43
3:A:82:ALA:HA	3:A:83:PRO:HD3	1.72	0.43
3:A:66:TYR:HD2	3:A:71:LEU:HD21	1.84	0.43
3:A:46:VAL:HG13	3:A:84:CYS:O	2.18	0.43
3:A:559:LYS:HE3	3:A:559:LYS:HB3	1.78	0.43
3:A:37:VAL:HG21	3:A:91:THR:HG23	1.99	0.43
1:B:902:DC:H2'	1:B:902:DC:H6	1.71	0.43
3:A:65:ILE:HG12	3:A:130:VAL:HG12	2.00	0.43
3:A:497:LYS:O	3:A:501:PRO:HB3	2.19	0.43
1:B:914:DC:H2''	1:B:915:DT:C7	2.48	0.43
3:A:171:ASP:HB2	3:A:173:GLN:CD	2.39	0.43
3:A:167:THR:HA	3:A:275:LEU:HD11	2.00	0.43
3:A:479:ILE:HG12	3:A:531:GLN:HE22	1.82	0.43
3:A:401:LEU:CD1	3:A:404:VAL:HB	2.49	0.43
3:A:324:LYS:C	3:A:326:GLU:N	2.72	0.43
3:A:525:LYS:O	3:A:527:ASN:N	2.47	0.43
3:A:48:GLU:O	3:A:52:GLN:HB2	2.19	0.43
2:C:934:DT:H6	4:C:701:HOH:O	2.02	0.42
3:A:500:ASN:ND2	3:A:502:ASN:CG	2.72	0.42
3:A:185:GLY:O	3:A:187:SER:N	2.50	0.42
3:A:379:ARG:HG2	3:A:380:GLY:N	2.34	0.42
3:A:388:SER:O	3:A:392:GLU:HG3	2.19	0.42
3:A:208:MET:HA	3:A:209:PRO:HD3	1.86	0.42
3:A:65:ILE:HA	3:A:130:VAL:HG12	2.00	0.42
3:A:496:ASN:O	3:A:499:ILE:O	2.37	0.42
3:A:65:ILE:HG12	3:A:130:VAL:HG11	2.00	0.42
3:A:500:ASN:O	3:A:502:ASN:N	2.53	0.42
3:A:558:ILE:HD12	3:A:563:LEU:CG	2.49	0.42
3:A:247:PHE:HA	4:A:769:HOH:O	2.17	0.42
3:A:50:LYS:NZ	4:A:692:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:923:DG:H2''	2:C:924:DA:H8	1.85	0.42
3:A:460:ILE:O	3:A:461:ASP:C	2.57	0.42
3:A:11:VAL:HG12	3:A:14:PRO:HG2	2.01	0.42
3:A:4:LYS:HB3	3:A:5:ILE:H	1.64	0.42
3:A:558:ILE:HD11	3:A:563:LEU:HG	2.01	0.42
3:A:534:ARG:HG2	3:A:538:ILE:HD11	2.02	0.42
3:A:422:ARG:HG3	3:A:423:ILE:N	2.35	0.42
3:A:460:ILE:CG1	3:A:569:ARG:NH2	2.82	0.42
3:A:101:TYR:N	3:A:101:TYR:CD1	2.87	0.42
3:A:378:ASN:HD22	3:A:378:ASN:N	2.17	0.42
3:A:503:GLU:O	3:A:506:LYS:HB2	2.19	0.42
3:A:359:GLU:HG2	3:A:368:LYS:HG3	2.02	0.41
3:A:304:GLU:O	3:A:308:THR:CG2	2.67	0.41
1:B:901:DT:H2'	1:B:902:DC:C4	2.55	0.41
3:A:390:LEU:HD12	3:A:394:LYS:HD2	2.01	0.41
3:A:67:THR:HA	3:A:128:SER:HA	2.02	0.41
3:A:517:PHE:CZ	3:A:535:LEU:HB3	2.56	0.41
3:A:163:ILE:HD13	3:A:163:ILE:HA	1.95	0.41
1:B:914:DC:H2'	1:B:915:DT:H72	2.02	0.41
3:A:375:VAL:HG23	4:A:663:HOH:O	2.20	0.41
3:A:61:GLN:HB2	4:A:721:HOH:O	2.20	0.41
3:A:397:LEU:HD22	4:A:747:HOH:O	2.21	0.41
3:A:158:SER:HB2	3:A:290:ARG:HH22	1.84	0.41
3:A:409:ILE:O	3:A:409:ILE:HG22	2.21	0.41
3:A:290:ARG:HD2	4:A:688:HOH:O	2.19	0.41
3:A:145:SER:HB2	3:A:148:GLU:H	1.84	0.41
3:A:22:ARG:HH12	3:A:91:THR:CG2	2.32	0.41
3:A:19:ASN:HD22	3:A:92:ILE:HG23	1.85	0.41
3:A:24:VAL:O	3:A:27:PHE:HB2	2.20	0.41
3:A:186:PHE:CE2	3:A:310:ARG:HD3	2.56	0.41
3:A:440:GLY:O	3:A:441:LYS:HG3	2.21	0.41
3:A:529:LYS:HD2	3:A:574:ASN:O	2.21	0.41
3:A:453:ILE:HG21	3:A:453:ILE:HD13	1.76	0.41
3:A:485:MET:HG3	3:A:519:PHE:CZ	2.56	0.40
3:A:432:PHE:CE1	3:A:551:LEU:HD21	2.56	0.40
3:A:136:LEU:HD22	3:A:140:LYS:NZ	2.35	0.40
1:B:906:DT:H2''	1:B:907:DG:C8	2.56	0.40
3:A:364:PHE:CD1	3:A:364:PHE:N	2.89	0.40
3:A:292:TYR:HE2	4:A:688:HOH:O	2.03	0.40
3:A:462:TYR:CZ	3:A:569:ARG:HB3	2.56	0.40
3:A:316:ILE:N	3:A:316:ILE:CD1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:DG:H2"	1:B:908:DA:OP2	2.21	0.40
3:A:420:GLN:NE2	4:A:676:HOH:O	2.53	0.40
2:C:935:DC:OP2	3:A:112:ARG:NH2	2.52	0.40
2:C:939:DC:H2"	2:C:940:DG:N7	2.36	0.40
3:A:391:GLU:HA	3:A:394:LYS:HD3	2.03	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	
3	A	562/576 (98%)	489 (87%)	61 (11%)	12 (2%)	9	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	526	GLY
3	A	528	TYR
3	A	278	ALA
3	A	461	ASP
3	A	553	ILE
3	A	320	ALA
3	A	501	PRO
3	A	215	ILE
3	A	304	GLU
3	A	322	SER
3	A	456	VAL
3	A	213	GLY

5.3.2 Protein sidechains ⓘ

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
3	A	490/500 (98%)	437 (89%)	53 (11%)	8 23

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	4	LYS
3	A	11	VAL
3	A	44	THR
3	A	47	LYS
3	A	49	SER
3	A	52	GLN
3	A	79	ARG
3	A	97	ASN
3	A	99	LYS
3	A	102	ILE
3	A	117	LEU
3	A	126	SER
3	A	134	VAL
3	A	156	ILE
3	A	169	LEU
3	A	174	HIS
3	A	184	LEU
3	A	187	SER
3	A	193	THR
3	A	195	LEU
3	A	203	THR
3	A	206	ASN
3	A	211	ASP
3	A	219	TRP
3	A	229	MET
3	A	256	ASP
3	A	275	LEU
3	A	292	TYR
3	A	293	TRP
3	A	308	THR

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Mol	Chain	Res	Type
3	A	314	LEU
3	A	316	ILE
3	A	330	ASP
3	A	354	THR
3	A	390	LEU
3	A	393	LYS
3	A	401	LEU
3	A	422	ARG
3	A	453	ILE
3	A	472	SER
3	A	487	ARG
3	A	500	ASN
3	A	511	SER
3	A	514	GLU
3	A	518	LEU
3	A	531	GLN
3	A	533	THR
3	A	535	LEU
3	A	546	LEU
3	A	548	VAL
3	A	551	LEU
3	A	562	THR
3	A	569	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	35	ASN
3	A	124	ASN
3	A	174	HIS
3	A	329	GLN
3	A	366	GLN
3	A	378	ASN
3	A	420	GLN
3	A	492	ASN
3	A	500	ASN
3	A	574	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.