



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 PM UTC

PDB ID : 1I7D / pdb_00001i7d
Title : NONCOVALENT COMPLEX OF E.COLI DNA TOPOISOMERASE III
WITH AN 8-BASE SINGLE-STRANDED DNA OLIGONUCLEOTIDE
Authors : Changela, A.; DiGate, R.J.; Mondragon, A.
Deposited on : 2001-03-08
Resolution : 2.05 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

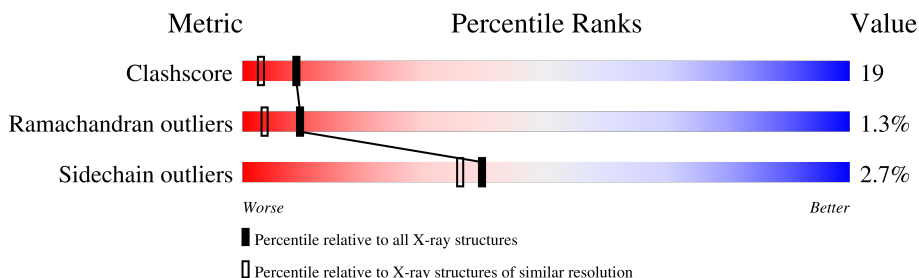
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	8	25% 38% 38%
2	A	659	63% 28% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5429 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 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			158	77	28	46	7			

- Molecule 2 is a protein called DNA TOPOISOMERASE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	620	Total	C	N	O	S	0	0	0
			4933	3119	892	902	20			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	PHE	TYR	engineered mutation	UNP P14294
A	654	HIS	-	expression tag	UNP P14294
A	655	HIS	-	expression tag	UNP P14294
A	656	HIS	-	expression tag	UNP P14294
A	657	HIS	-	expression tag	UNP P14294
A	658	HIS	-	expression tag	UNP P14294
A	659	HIS	-	expression tag	UNP P14294

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	25	Total	O	0	0
			25	25		
5	A	307	Total	O	0	0
			307	307		

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. 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. 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.

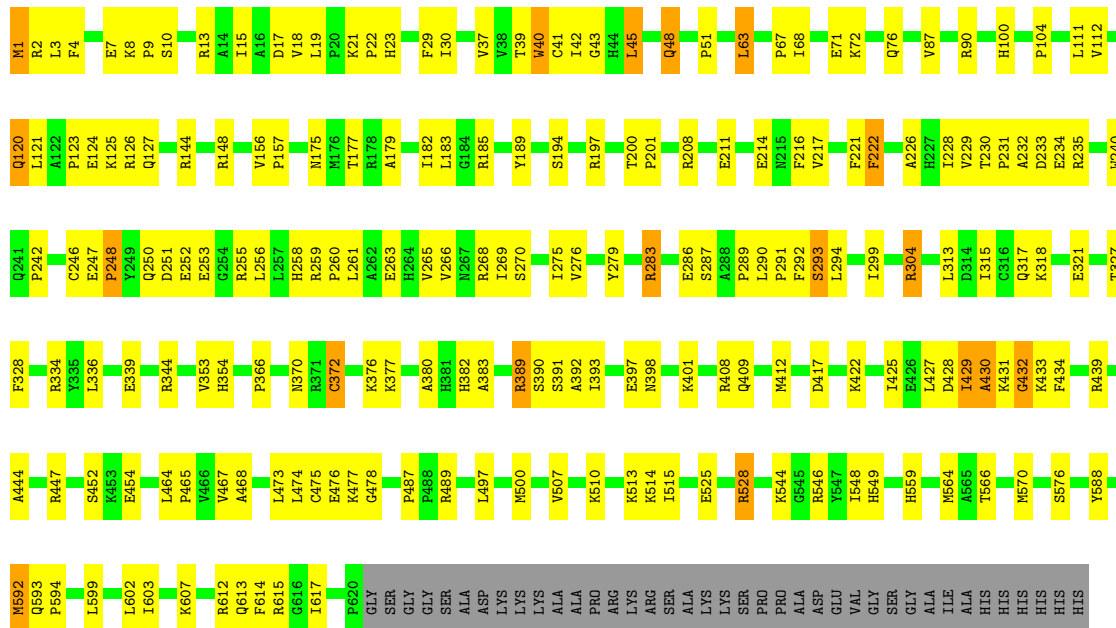
- Molecule 1: 5'-D(*CP*GP*CP*AP*AP*CP*TP*T)-3'

Chain B: 



- Molecule 2: DNA TOPOISOMERASE III

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.01Å 60.83Å 125.36Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	29.63 – 2.05	Depositor
% Data completeness (in resolution range)	96.1 (29.63-2.05)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	9.00	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5429	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.36	0/176	1.09	2/269 (0.7%)
2	A	0.39	0/5040	0.87	11/6835 (0.2%)
All	All	0.39	0/5216	0.88	13/7104 (0.2%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	293	SER	N-CA-C	-7.09	99.44	110.42
2	A	40	TRP	N-CA-C	6.71	118.72	108.52
2	A	292	PHE	N-CA-C	6.51	119.92	110.28
2	A	592	MET	N-CA-C	6.36	118.29	111.36
2	A	546	ARG	N-CA-C	-6.24	105.31	113.17
2	A	43	GLY	N-CA-C	-5.90	101.96	112.22
2	A	175	ASN	N-CA-C	5.57	117.44	111.36
2	A	71	GLU	N-CA-C	-5.41	104.80	111.40
1	B	708	DT	C2'-C3'-O3'	-5.25	103.63	111.50
2	A	304	ARG	N-CA-C	5.19	116.75	111.14
1	B	707	DT	N1-C1'-C2'	-5.16	105.75	113.50
2	A	528	ARG	N-CA-C	5.10	117.23	111.11
2	A	45	LEU	N-CA-C	-5.08	107.25	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	705	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	158	0	92	17	0
2	A	4933	0	4954	173	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
5	A	307	0	0	14	0
5	B	25	0	0	3	0
All	All	5429	0	5046	189	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 19.

All (189) 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:B:706:DC:C2'	1:B:707:DT:H5''	1.76	1.15
2:A:564:MET:HE1	2:A:602:LEU:HD11	1.35	1.06
1:B:707:DT:H5'	1:B:707:DT:H6	1.24	1.03
1:B:706:DC:H2'	1:B:707:DT:H5''	1.47	0.95
2:A:612:ARG:HD2	2:A:613:GLN:N	1.84	0.92
2:A:467:VAL:HG12	2:A:468:ALA:H	1.37	0.89
2:A:144:ARG:HE	2:A:148:ARG:CZ	1.87	0.88
2:A:422:LYS:HG2	2:A:439:ARG:HG2	1.58	0.85
1:B:706:DC:H2''	1:B:707:DT:H5''	1.58	0.84
2:A:612:ARG:HD2	2:A:613:GLN:H	1.40	0.81
2:A:428:ASP:HA	2:A:432:GLY:HA3	1.62	0.81
2:A:612:ARG:NH1	2:A:613:GLN:HB3	1.98	0.78
2:A:124:GLU:HG3	2:A:125:LYS:H	1.49	0.77
2:A:276:VAL:HG21	2:A:467:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:GLN:HE21	2:A:120:GLN:HA	1.53	0.73
2:A:48:GLN:HG3	5:A:1114:HOH:O	1.88	0.73
2:A:258:HIS:CD2	2:A:260:PRO:HD2	2.23	0.72
1:B:707:DT:H5'	1:B:707:DT:C6	2.16	0.72
1:B:706:DC:H2'	1:B:707:DT:C5'	2.20	0.71
2:A:339:GLU:HG3	5:A:997:HOH:O	1.90	0.71
2:A:429:ILE:H	2:A:432:GLY:CA	2.03	0.70
2:A:269:ILE:HG22	2:A:429:ILE:HG21	1.74	0.70
2:A:376:LYS:HD2	5:A:1185:HOH:O	1.91	0.70
2:A:247:GLU:HB3	2:A:248:PRO:HD3	1.74	0.68
2:A:612:ARG:HH11	2:A:613:GLN:HB3	1.57	0.68
2:A:515:ILE:HD13	2:A:576:SER:HB3	1.76	0.68
2:A:124:GLU:HG3	2:A:125:LYS:N	2.10	0.66
1:B:704:DA:N3	5:B:2:HOH:O	2.27	0.66
2:A:259:ARG:HB3	2:A:260:PRO:HD3	1.77	0.66
2:A:67:PRO:HG3	2:A:603:ILE:HG13	1.78	0.65
1:B:708:DT:H3'	2:A:321:GLU:OE1	1.96	0.64
1:B:704:DA:H2''	1:B:705:DA:H5'	1.80	0.63
1:B:706:DC:C2'	1:B:707:DT:C5'	2.68	0.63
2:A:144:ARG:HE	2:A:148:ARG:NH2	1.97	0.63
2:A:291:PRO:HD2	2:A:334:ARG:O	1.98	0.62
2:A:428:ASP:HA	2:A:432:GLY:CA	2.29	0.62
2:A:279:TYR:HD1	2:A:425:ILE:HG12	1.64	0.62
2:A:7:GLU:HG3	2:A:111:LEU:HD13	1.80	0.62
2:A:283:ARG:HD2	2:A:283:ARG:H	1.64	0.62
2:A:208:ARG:NH2	2:A:566:THR:O	2.33	0.62
2:A:429:ILE:H	2:A:432:GLY:HA2	1.62	0.62
1:B:707:DT:H6	1:B:707:DT:C5'	2.06	0.62
2:A:467:VAL:HG12	2:A:468:ALA:N	2.10	0.62
2:A:63:LEU:HD13	2:A:182:ILE:HG21	1.80	0.61
2:A:260:PRO:O	2:A:263:GLU:HG2	2.01	0.61
2:A:354:HIS:HE1	2:A:389:ARG:O	1.83	0.60
2:A:489:ARG:HB2	2:A:489:ARG:NH1	2.16	0.60
2:A:144:ARG:HH21	2:A:148:ARG:HH12	1.48	0.60
2:A:240:TRP:HB2	2:A:434:PHE:CE1	2.37	0.60
2:A:2:ARG:HD3	2:A:4:PHE:CE1	2.36	0.60
2:A:392:ALA:C	2:A:393:ILE:HD12	2.27	0.60
2:A:615:ARG:HH11	2:A:615:ARG:HG2	1.67	0.59
2:A:123:PRO:HA	2:A:126:ARG:NH1	2.18	0.58
2:A:477:LYS:HG2	2:A:478:GLY:N	2.18	0.58
2:A:429:ILE:O	2:A:430:ALA:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:510:LYS:HE2	2:A:514:LYS:NZ	2.20	0.57
2:A:275:ILE:HB	2:A:428:ASP:HB3	1.87	0.56
2:A:72:LYS:HE3	5:A:1045:HOH:O	2.06	0.56
2:A:392:ALA:O	2:A:393:ILE:HD12	2.05	0.56
2:A:144:ARG:HE	2:A:148:ARG:NH1	2.02	0.56
2:A:500:MET:HE2	2:A:528:ARG:HG2	1.86	0.56
2:A:474:LEU:HD22	2:A:475:CYS:N	2.21	0.56
2:A:200:THR:HB	2:A:201:PRO:HD3	1.87	0.55
2:A:41:CYS:HB3	2:A:45:LEU:HG	1.89	0.54
2:A:123:PRO:O	2:A:127:GLN:HG2	2.07	0.54
2:A:588:TYR:CZ	2:A:592:MET:HG3	2.41	0.54
2:A:444:ALA:O	2:A:447:ARG:HB2	2.07	0.54
2:A:614:PHE:O	2:A:617:ILE:HG12	2.08	0.54
2:A:261:LEU:O	2:A:265:VAL:HG23	2.09	0.53
2:A:489:ARG:HD3	5:A:1084:HOH:O	2.08	0.53
2:A:123:PRO:HA	2:A:126:ARG:HH12	1.73	0.52
2:A:299:ILE:HG13	2:A:497:LEU:HD23	1.91	0.52
2:A:327:THR:O	2:A:328:PHE:C	2.52	0.52
2:A:8:LYS:HE3	5:A:1086:HOH:O	2.10	0.52
2:A:428:ASP:CA	2:A:432:GLY:HA3	2.38	0.52
2:A:382:HIS:HD2	2:A:383:ALA:O	1.93	0.52
2:A:431:LYS:HG3	2:A:433:LYS:HG2	1.90	0.51
1:B:704:DA:H2''	1:B:705:DA:C5'	2.39	0.51
2:A:276:VAL:HG21	2:A:467:VAL:CG1	2.38	0.51
2:A:429:ILE:HG22	2:A:430:ALA:H	1.74	0.51
2:A:474:LEU:HD22	2:A:475:CYS:H	1.74	0.51
2:A:226:ALA:HB2	2:A:269:ILE:HD12	1.92	0.51
2:A:87:VAL:HA	2:A:90:ARG:NH1	2.25	0.51
2:A:269:ILE:HG22	2:A:429:ILE:CG2	2.40	0.51
2:A:269:ILE:CG2	2:A:429:ILE:HG21	2.39	0.51
2:A:291:PRO:HB2	2:A:383:ALA:CB	2.40	0.51
2:A:315:ILE:HD13	2:A:398:ASN:HB3	1.93	0.51
2:A:293:SER:HB3	2:A:334:ARG:HG2	1.92	0.51
2:A:240:TRP:O	2:A:242:PRO:HD3	2.10	0.51
1:B:707:DT:H2'	1:B:708:DT:C6	2.45	0.50
2:A:230:THR:HB	2:A:234:GLU:HB2	1.93	0.50
2:A:217:VAL:O	2:A:217:VAL:HG23	2.11	0.50
1:B:705:DA:H2''	1:B:706:DC:H5''	1.95	0.49
2:A:179:ALA:O	2:A:183:LEU:HG	2.11	0.49
2:A:473:LEU:HD12	2:A:473:LEU:N	2.27	0.49
2:A:228:ILE:HG13	2:A:427:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:570:MET:HE2	5:A:999:HOH:O	2.11	0.49
2:A:229:VAL:HG12	2:A:474:LEU:O	2.12	0.49
2:A:76:GLN:NE2	5:A:1190:HOH:O	2.46	0.48
2:A:276:VAL:HG22	2:A:427:LEU:CD2	2.43	0.48
2:A:21:LYS:HB3	2:A:22:PRO:HA	1.95	0.48
2:A:279:TYR:CD1	2:A:425:ILE:HG12	2.45	0.48
2:A:228:ILE:HG13	2:A:427:LEU:HD12	1.96	0.48
2:A:454:GLU:HG3	5:A:1157:HOH:O	2.14	0.48
2:A:251:ASP:OD1	2:A:252:GLU:N	2.37	0.48
2:A:564:MET:HE1	2:A:602:LEU:CD1	2.26	0.48
2:A:289:PRO:HB2	2:A:409:GLN:NE2	2.29	0.48
2:A:9:PRO:HG3	2:A:40:TRP:NE1	2.29	0.47
2:A:429:ILE:O	2:A:430:ALA:C	2.56	0.47
2:A:234:GLU:HB3	2:A:465:PRO:CG	2.44	0.47
2:A:1:MET:HE2	2:A:37:VAL:HG21	1.96	0.47
2:A:474:LEU:C	2:A:474:LEU:HD13	2.39	0.47
2:A:507:VAL:O	2:A:513:LYS:HE2	2.14	0.47
2:A:189:TYR:CD1	2:A:617:ILE:HG13	2.50	0.47
2:A:253:GLU:HG3	2:A:255:ARG:HH12	1.79	0.47
1:B:708:DT:H71	5:B:278:HOH:O	2.14	0.47
2:A:294:LEU:HD21	2:A:313:LEU:HD13	1.96	0.47
2:A:315:ILE:CD1	2:A:398:ASN:HB3	2.45	0.47
2:A:15:ILE:O	2:A:19:LEU:HG	2.15	0.47
2:A:104:PRO:HG2	2:A:380:ALA:HA	1.97	0.47
2:A:467:VAL:CG1	2:A:468:ALA:H	2.19	0.46
2:A:593:GLN:HB2	2:A:594:PRO:HD3	1.97	0.46
2:A:428:ASP:OD1	2:A:432:GLY:HA3	2.15	0.46
2:A:431:LYS:O	2:A:433:LYS:N	2.48	0.46
2:A:72:LYS:HA	2:A:72:LYS:HD2	1.72	0.46
1:B:702:DG:H2'	1:B:702:DG:N3	2.30	0.46
2:A:90:ARG:HD2	5:A:1028:HOH:O	2.15	0.46
2:A:10:SER:HA	2:A:13:ARG:NH1	2.31	0.46
1:B:706:DC:C3'	1:B:707:DT:H5''	2.43	0.46
2:A:100:HIS:NE2	2:A:112:VAL:HB	2.31	0.46
2:A:230:THR:CB	2:A:234:GLU:HB2	2.45	0.46
2:A:304:ARG:NH1	5:A:1154:HOH:O	2.48	0.46
2:A:185:ARG:HG3	2:A:185:ARG:HH11	1.82	0.45
2:A:144:ARG:NE	2:A:148:ARG:NH2	2.62	0.45
2:A:397:GLU:HG3	5:A:941:HOH:O	2.16	0.45
2:A:100:HIS:CE1	2:A:112:VAL:HB	2.52	0.45
2:A:228:ILE:HG22	2:A:229:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:PRO:C	2:A:233:ASP:H	2.24	0.45
2:A:377:LYS:NZ	5:A:985:HOH:O	2.49	0.45
2:A:221:PHE:CG	2:A:255:ARG:HD3	2.52	0.45
2:A:242:PRO:HB2	2:A:250:GLN:NE2	2.31	0.45
2:A:286:GLU:CD	2:A:447:ARG:HH21	2.26	0.44
2:A:121:LEU:HG	2:A:125:LYS:HB2	1.98	0.44
2:A:235:ARG:HH11	2:A:235:ARG:HG3	1.82	0.44
2:A:144:ARG:NH2	2:A:148:ARG:HH12	2.14	0.44
2:A:216:PHE:CD2	2:A:487:PRO:HG3	2.53	0.44
2:A:336:LEU:HD12	2:A:372:CYS:SG	2.58	0.44
2:A:67:PRO:HG3	2:A:603:ILE:CG1	2.48	0.44
2:A:3:LEU:HD11	2:A:39:THR:HG22	1.99	0.44
2:A:230:THR:HG22	2:A:232:ALA:H	1.82	0.43
2:A:344:ARG:NE	2:A:366:PRO:O	2.50	0.43
2:A:41:CYS:HB2	2:A:111:LEU:HD21	2.01	0.43
2:A:222:PHE:N	2:A:222:PHE:CD1	2.86	0.43
2:A:229:VAL:O	2:A:473:LEU:HB3	2.19	0.43
2:A:268:ARG:HH21	2:A:430:ALA:HB1	1.84	0.43
2:A:391:SER:O	2:A:393:ILE:HD13	2.19	0.43
2:A:464:LEU:HA	2:A:465:PRO:HD3	1.85	0.43
2:A:474:LEU:HD13	2:A:476:GLU:N	2.34	0.43
2:A:120:GLN:HE21	2:A:120:GLN:CA	2.20	0.43
2:A:29:PHE:O	2:A:30:ILE:HD13	2.18	0.43
2:A:177:THR:HG23	2:A:194:SER:HA	2.01	0.43
2:A:51:PRO:HB3	2:A:68:ILE:HD13	2.01	0.42
2:A:197:ARG:O	2:A:201:PRO:HG2	2.19	0.42
5:B:74:HOH:O	2:A:328:PHE:HE2	2.02	0.42
2:A:42:ILE:H	2:A:45:LEU:HD21	1.85	0.42
2:A:156:VAL:HB	2:A:157:PRO:HD3	2.01	0.42
2:A:287:SER:HA	2:A:417:ASP:OD1	2.19	0.42
2:A:289:PRO:HB2	2:A:409:GLN:HE22	1.84	0.42
2:A:354:HIS:CE1	2:A:389:ARG:O	2.69	0.42
2:A:489:ARG:HH11	2:A:489:ARG:CB	2.32	0.42
2:A:353:VAL:HG11	2:A:390:SER:O	2.20	0.42
2:A:266:VAL:HG13	2:A:478:GLY:HA3	2.01	0.42
2:A:397:GLU:O	2:A:401:LYS:HG3	2.21	0.41
2:A:603:ILE:HG22	2:A:607:LYS:HE3	2.01	0.41
2:A:408:ARG:O	2:A:412:MET:HG3	2.21	0.41
2:A:559:HIS:HD2	5:A:1061:HOH:O	2.03	0.41
2:A:290:LEU:HB3	2:A:291:PRO:CD	2.50	0.41
2:A:500:MET:CE	2:A:528:ARG:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:246:CYS:O	2:A:250:GLN:HG3	2.21	0.41
2:A:230:THR:O	2:A:233:ASP:N	2.54	0.41
2:A:253:GLU:HG3	2:A:255:ARG:NH1	2.36	0.41
2:A:548:ILE:C	2:A:549:HIS:HD2	2.28	0.41
2:A:234:GLU:HB3	2:A:465:PRO:HG3	2.03	0.41
2:A:256:LEU:HD11	2:A:261:LEU:HD23	2.02	0.40
2:A:19:LEU:O	2:A:23:HIS:HE1	2.05	0.40
2:A:229:VAL:HA	2:A:234:GLU:O	2.21	0.40
2:A:525:GLU:OE2	2:A:525:GLU:HA	2.21	0.40
2:A:63:LEU:O	2:A:607:LYS:HE2	2.22	0.40
2:A:15:ILE:O	2:A:18:VAL:HG22	2.22	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
2	A	618/659 (94%)	583 (94%)	27 (4%)	8 (1%)	9 3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	430	ALA
2	A	432	GLY
2	A	452	SER
2	A	270	SER
2	A	544	LYS
2	A	370	ASN
2	A	248	PRO
2	A	429	ILE

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	
2	A	528/555 (95%)	514 (97%)	14 (3%)	39	36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1	MET
2	A	17	ASP
2	A	48	GLN
2	A	63	LEU
2	A	120	GLN
2	A	211	GLU
2	A	214	GLU
2	A	222	PHE
2	A	283	ARG
2	A	317	GLN
2	A	318	LYS
2	A	372	CYS
2	A	389	ARG
2	A	599	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	HIS
2	A	34	ASN
2	A	74	GLN
2	A	76	GLN
2	A	120	GLN
2	A	130	GLN
2	A	138	ASN
2	A	250	GLN
2	A	272	GLN
2	A	311	ASN
2	A	323	HIS

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Mol	Chain	Res	Type
2	A	345	HIS
2	A	354	HIS
2	A	370	ASN
2	A	382	HIS
2	A	398	ASN
2	A	409	GLN
2	A	413	GLN
2	A	484	GLN
2	A	490	HIS
2	A	549	HIS
2	A	580	GLN
2	A	605	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	SO4	A	900	-	4,4,4	0.39	0	6,6,6	0.09	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.