Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 09:53 PM EDT

PDB ID	:	4XR0
Title	:	Escherichia Coli Replication Terminator Protein (Tus) Complexed With DNA-G/T mismatch.
Authors	:	Oakley, A.J.
Deposited on	:	2015-01-20
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

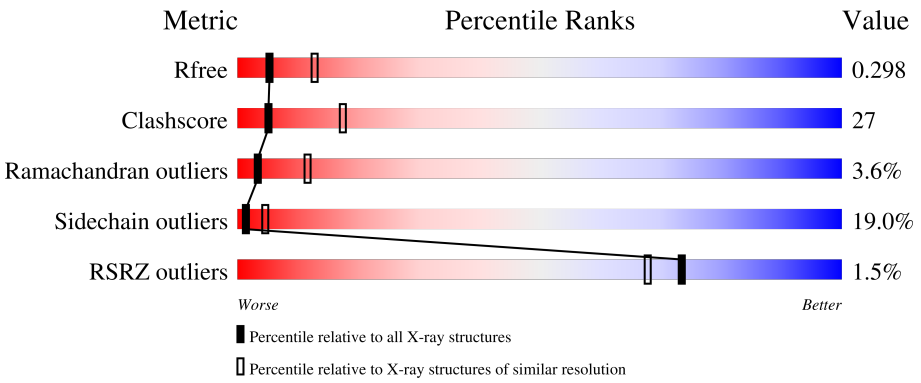
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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 <=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	316	2%, 49%, 37%, 10%, • •
2	B	16	44%, 44%, 6%, 6%
3	C	16	12%, 81%, 6%

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
4	IOD	A	1005	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3125 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 DNA replication terminus site-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	2504	1590	469	442	3	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P16525
A	-5	HIS	-	expression tag	UNP P16525
A	-4	HIS	-	expression tag	UNP P16525
A	-3	HIS	-	expression tag	UNP P16525
A	-2	HIS	-	expression tag	UNP P16525
A	-1	HIS	-	expression tag	UNP P16525
A	0	HIS	-	expression tag	UNP P16525

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	15	289	138	54	83	14	0	0	0

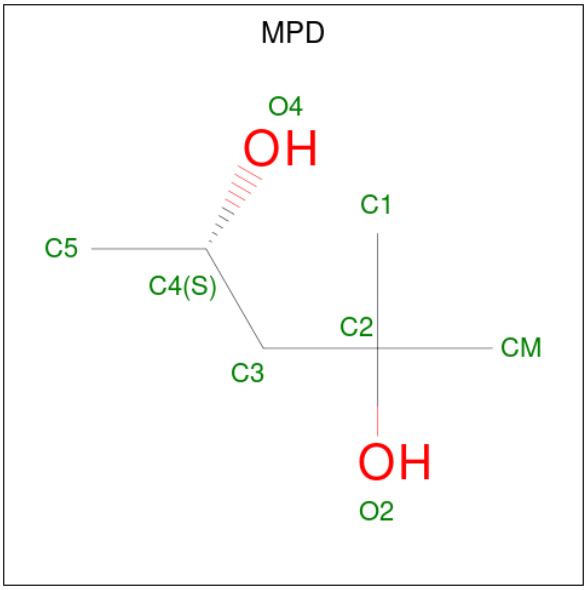
- Molecule 3 is a DNA chain called DNA (5'-D(*AP*TP*TP*AP*TP*GP*TP*TP*GP*TP*AP*AP*CP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	15	288	139	47	88	14	0	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total I 5 5	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 8 6 2	0	0

- Molecule 6 is water.

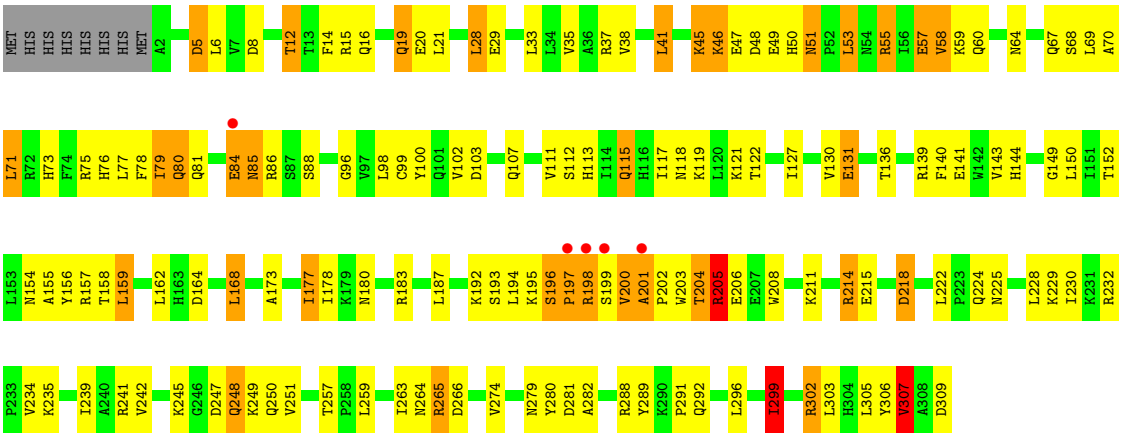
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	2	Total O 2 2	0	0
6	C	6	Total O 6 6	0	0

3 Residue-property plots (i)

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.

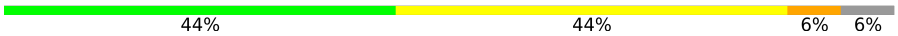
• Molecule 1: DNA replication terminus site-binding protein

Chain A:



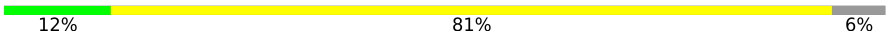
• Molecule 2: DNA (5'-D(*AP*GP*TP*TP*AP*CP*AP*AP*CP*AP*TP*AP*GP*T)-3')

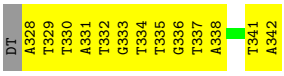
Chain B:



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

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.52Å 64.52Å 248.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.45 – 2.80 44.87 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.5 (62.45-2.80) 97.5 (44.87-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.98 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.218 , 0.296 0.217 , 0.298	Depositor DCC
R_{free} test set	682 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3125	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: IOD, MPD

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	0.85	0/2562	1.08	6/3479 (0.2%)
2	B	0.87	1/324 (0.3%)	1.12	2/499 (0.4%)
3	C	0.62	0/321	1.13	1/495 (0.2%)
All	All	0.84	1/3207 (0.0%)	1.09	9/4473 (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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	320	DC	O3'-P	-7.66	1.51	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	317	DC	C1'-O4'-C4'	-7.14	102.96	110.10
1	A	307	VAL	CB-CA-C	-6.57	98.93	111.40
2	B	323	DA	O5'-P-OP1	-6.02	100.28	105.70
1	A	168	LEU	CB-CG-CD1	-5.70	101.31	111.00
1	A	218	ASP	CB-CG-OD2	-5.70	113.17	118.30
3	C	338	DA	C1'-O4'-C4'	-5.66	104.44	110.10
1	A	302	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	218	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	299	ILE	CB-CA-C	-5.07	101.46	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	THR	Peptide

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	2504	0	2531	141	0
2	B	289	0	159	11	0
3	C	288	0	162	19	0
4	A	5	0	0	4	0
5	B	8	0	14	1	0
6	A	23	0	0	2	0
6	B	2	0	0	0	0
6	C	6	0	0	3	0
All	All	3125	0	2866	159	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 27.

All (159) 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:265:ARG:HG2	1:A:265:ARG:HH11	1.07	1.15
1:A:232:ARG:NH1	4:A:1003:IOD:I	2.62	1.02
1:A:241:ARG:HD2	1:A:250:GLN:NE2	1.73	1.02
1:A:224:GLN:HG2	4:A:1005:IOD:I	2.34	0.96
2:B:324:DG:C8	3:C:329:DT:O4	2.21	0.94
1:A:200:VAL:HG11	1:A:208:TRP:CE3	2.02	0.93
1:A:180:ASN:ND2	1:A:229:LYS:HE2	1.89	0.88
1:A:265:ARG:HH11	1:A:265:ARG:CG	1.89	0.85
1:A:177:ILE:HD12	1:A:178:ILE:N	1.90	0.85
1:A:265:ARG:HG2	1:A:265:ARG:NH1	1.82	0.84
1:A:241:ARG:HD2	1:A:250:GLN:HE22	1.41	0.82
3:C:330:DT:H2"	3:C:331:DA:O5'	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:O	1:A:155:ALA:HB3	1.83	0.78
1:A:55:ARG:HH11	1:A:55:ARG:CG	1.97	0.77
1:A:247:ASP:O	1:A:249:LYS:N	2.17	0.76
1:A:46:LYS:HG3	1:A:49:GLU:OE1	1.85	0.76
1:A:78:PHE:H	1:A:81:GLN:HE22	1.29	0.76
1:A:168:LEU:HD11	1:A:242:VAL:HG22	1.68	0.75
1:A:51:ASN:ND2	1:A:51:ASN:H	1.85	0.74
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.69	0.74
1:A:55:ARG:HH11	1:A:55:ARG:HG2	1.51	0.73
1:A:37:ARG:HH11	1:A:60:GLN:HE22	1.33	0.73
1:A:177:ILE:HD12	1:A:177:ILE:C	2.08	0.73
2:B:324:DG:N7	3:C:329:DT:O4	2.20	0.73
1:A:139:ARG:O	1:A:143:VAL:HG23	1.89	0.72
1:A:78:PHE:H	1:A:81:GLN:NE2	1.88	0.72
1:A:88:SER:OG	2:B:323:DA:OP1	2.06	0.72
1:A:288:ARG:NH2	2:B:312:DA:H5'	2.06	0.71
1:A:140:PHE:O	1:A:144:HIS:HD2	1.75	0.69
1:A:16:GLN:O	1:A:20:GLU:HG2	1.93	0.68
1:A:203:TRP:CZ2	1:A:211:LYS:HE3	2.28	0.68
1:A:180:ASN:HD22	1:A:229:LYS:HE2	1.56	0.68
1:A:12:THR:HG23	1:A:16:GLN:HE21	1.60	0.67
1:A:127:ILE:HA	1:A:131:GLU:HB2	1.77	0.67
3:C:329:DT:OP2	3:C:329:DT:O2	2.13	0.67
1:A:288:ARG:HD2	2:B:311:DT:O2	1.96	0.66
1:A:201:ALA:CB	1:A:202:PRO:HD3	2.25	0.66
1:A:241:ARG:CD	1:A:250:GLN:NE2	2.55	0.66
1:A:19:GLN:HE21	1:A:19:GLN:HA	1.62	0.64
1:A:197:PRO:HG2	1:A:198:ARG:H	1.63	0.64
1:A:214:ARG:NH1	1:A:218:ASP:OD1	2.28	0.64
1:A:80:GLN:HE22	1:A:149:GLY:HA3	1.63	0.64
1:A:180:ASN:ND2	1:A:229:LYS:CE	2.62	0.63
3:C:336:DG:H2"	3:C:337:DT:O5'	1.99	0.63
1:A:51:ASN:HD22	1:A:51:ASN:N	1.97	0.62
1:A:241:ARG:HD2	1:A:250:GLN:HE21	1.59	0.62
1:A:198:ARG:CB	1:A:205:ARG:HA	2.30	0.61
1:A:12:THR:HG23	1:A:16:GLN:NE2	2.16	0.61
1:A:200:VAL:HG11	1:A:208:TRP:CZ3	2.35	0.61
1:A:55:ARG:CG	1:A:55:ARG:NH1	2.61	0.60
1:A:55:ARG:HH21	1:A:279:ASN:HD22	1.50	0.60
1:A:112:SER:HA	1:A:115:GLN:HG3	1.83	0.59
1:A:55:ARG:HH21	1:A:279:ASN:ND2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:HD21	1:A:229:LYS:NZ	2.00	0.59
1:A:51:ASN:ND2	1:A:51:ASN:N	2.47	0.59
1:A:67:GLN:NE2	1:A:100:TYR:OH	2.29	0.59
1:A:41:LEU:CD1	1:A:58:VAL:HG12	2.32	0.58
1:A:159:LEU:CD1	1:A:159:LEU:N	2.67	0.58
1:A:299:ILE:HD13	1:A:307:VAL:HG22	1.85	0.58
1:A:21:LEU:HD12	1:A:117:ILE:HD13	1.86	0.58
1:A:168:LEU:CD1	1:A:242:VAL:HG22	2.34	0.57
1:A:69:LEU:O	1:A:70:ALA:C	2.43	0.56
1:A:157:ARG:HB2	6:C:402:HOH:O	2.06	0.56
3:C:328:DA:H2"	3:C:329:DT:OP2	2.04	0.56
1:A:45:LYS:HE2	1:A:45:LYS:H	1.70	0.56
1:A:197:PRO:CG	1:A:198:ARG:H	2.19	0.55
1:A:102:VAL:O	1:A:264:ASN:HA	2.06	0.55
1:A:302:ARG:HD2	3:C:331:DA:P	2.47	0.55
1:A:48:ASP:HA	1:A:51:ASN:OD1	2.06	0.55
1:A:111:VAL:O	1:A:115:GLN:CG	2.55	0.55
1:A:264:ASN:OD1	1:A:266:ASP:HB2	2.07	0.54
1:A:140:PHE:O	1:A:144:HIS:CD2	2.59	0.54
1:A:180:ASN:HD21	1:A:229:LYS:CE	2.20	0.54
1:A:302:ARG:HD2	3:C:331:DA:OP2	2.06	0.54
1:A:211:LYS:O	1:A:215:GLU:HG3	2.08	0.54
1:A:203:TRP:CE2	1:A:211:LYS:HE3	2.42	0.53
1:A:111:VAL:O	1:A:115:GLN:HG3	2.08	0.53
1:A:50:HIS:CE1	3:C:332:DT:H4'	2.43	0.53
1:A:224:GLN:CG	4:A:1005:IOD:I	3.18	0.53
3:C:329:DT:H2"	3:C:330:DT:C6	2.44	0.53
1:A:264:ASN:OD1	1:A:266:ASP:N	2.39	0.53
1:A:201:ALA:HB3	1:A:202:PRO:CD	2.35	0.53
1:A:5:ASP:OD2	1:A:5:ASP:C	2.47	0.52
1:A:45:LYS:HE2	1:A:45:LYS:N	2.25	0.52
1:A:51:ASN:H	1:A:51:ASN:HD22	1.54	0.52
1:A:177:ILE:HD12	1:A:178:ILE:CA	2.39	0.52
3:C:328:DA:H2	6:C:404:HOH:O	1.93	0.52
1:A:48:ASP:HB3	1:A:51:ASN:OD1	2.10	0.51
3:C:329:DT:O2	3:C:329:DT:H2'	2.11	0.51
1:A:281:ASP:OD1	1:A:281:ASP:C	2.48	0.51
1:A:37:ARG:HH11	1:A:60:GLN:NE2	2.05	0.51
1:A:37:ARG:NH2	1:A:274:VAL:O	2.39	0.50
1:A:204:THR:O	1:A:206:GLU:N	2.43	0.50
1:A:117:ILE:O	1:A:121:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:CB	1:A:202:PRO:CD	2.90	0.50
1:A:55:ARG:NH2	1:A:279:ASN:ND2	2.59	0.50
1:A:76:HIS:HB3	6:A:1115:HOH:O	2.12	0.49
1:A:45:LYS:HD2	6:A:1120:HOH:O	2.11	0.49
1:A:118:ASN:HA	1:A:121:LYS:HG3	1.94	0.49
1:A:21:LEU:HD12	1:A:117:ILE:HG21	1.95	0.49
2:B:323:DA:H62	3:C:330:DT:H3	1.60	0.49
3:C:341:DT:H2"	6:C:405:HOH:O	2.13	0.49
1:A:154:ASN:HA	1:A:157:ARG:NE	2.28	0.49
1:A:45:LYS:HB3	1:A:47:GLU:OE2	2.13	0.49
1:A:299:ILE:CD1	1:A:307:VAL:HG22	2.42	0.49
1:A:79:ILE:HG13	1:A:80:GLN:HE21	1.79	0.48
1:A:14:PHE:O	1:A:15:ARG:C	2.51	0.47
1:A:159:LEU:N	1:A:159:LEU:HD13	2.28	0.47
1:A:288:ARG:NH2	2:B:312:DA:C5'	2.77	0.47
3:C:341:DT:H4'	3:C:342:DA:OP2	2.14	0.47
1:A:102:VAL:HG23	1:A:103:ASP:O	2.15	0.47
1:A:20:GLU:OE2	1:A:20:GLU:HA	2.15	0.47
1:A:162:LEU:HD11	1:A:259:LEU:HD13	1.97	0.47
1:A:296:LEU:HB3	1:A:306:TYR:HB3	1.96	0.47
1:A:73:HIS:CD2	1:A:257:THR:HG22	2.49	0.47
1:A:38:VAL:HG12	1:A:96:GLY:HA3	1.95	0.46
1:A:288:ARG:HH21	2:B:312:DA:C5'	2.29	0.46
1:A:289:TYR:CE2	1:A:291:PRO:HG3	2.51	0.46
1:A:50:HIS:CE1	3:C:333:DG:H5'	2.50	0.45
2:B:323:DA:H2'	2:B:323:DA:N3	2.31	0.45
1:A:103:ASP:OD1	1:A:103:ASP:C	2.53	0.45
2:B:313:DG:H1'	2:B:314:DT:C6	2.51	0.45
1:A:196:SER:CB	1:A:197:PRO:HD3	2.46	0.45
1:A:79:ILE:HG13	1:A:80:GLN:NE2	2.32	0.45
1:A:53:LEU:HD12	1:A:53:LEU:HA	1.62	0.45
1:A:130:VAL:O	1:A:131:GLU:C	2.51	0.45
3:C:328:DA:H2"	3:C:329:DT:O2	2.16	0.45
1:A:144:HIS:HE1	1:A:150:LEU:O	2.00	0.45
1:A:173:ALA:HB2	1:A:239:ILE:HD13	1.98	0.44
1:A:68:SER:O	1:A:69:LEU:C	2.54	0.44
5:B:401:MPD:O2	5:B:401:MPD:H53	2.18	0.44
1:A:33:LEU:HD12	1:A:99:CYS:O	2.17	0.44
1:A:76:HIS:HA	1:A:81:GLN:OE1	2.17	0.44
1:A:70:ALA:O	1:A:73:HIS:HB3	2.18	0.44
1:A:111:VAL:O	1:A:115:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:O	1:A:229:LYS:HB3	2.18	0.43
1:A:41:LEU:HA	1:A:41:LEU:HD12	1.69	0.43
1:A:71:LEU:O	1:A:75:ARG:HG3	2.18	0.43
1:A:28:LEU:HD21	1:A:100:TYR:CD2	2.54	0.42
1:A:299:ILE:H	1:A:299:ILE:HG12	1.64	0.42
1:A:84:GLU:C	1:A:86:ARG:N	2.72	0.42
1:A:168:LEU:HD13	1:A:168:LEU:HA	1.61	0.42
2:B:324:DG:H2'	2:B:324:DG:N3	2.33	0.42
1:A:302:ARG:HG2	1:A:302:ARG:HH11	1.84	0.42
1:A:241:ARG:CD	1:A:250:GLN:HE21	2.28	0.42
3:C:334:DT:H1'	3:C:335:DT:H5'	2.00	0.42
1:A:84:GLU:C	1:A:86:ARG:H	2.23	0.41
1:A:303:LEU:HA	1:A:303:LEU:HD23	1.82	0.41
1:A:280:TYR:CE2	1:A:282:ALA:HB2	2.55	0.41
1:A:50:HIS:HE1	3:C:332:DT:H4'	1.85	0.41
1:A:159:LEU:HD13	1:A:159:LEU:H	1.86	0.41
1:A:164:ASP:OD1	1:A:263:ILE:HA	2.20	0.41
1:A:203:TRP:CZ2	1:A:211:LYS:CE	3.02	0.41
1:A:241:ARG:HA	1:A:251:VAL:O	2.21	0.41
1:A:225:ASN:HB3	4:A:1005:IOD:I	2.91	0.41
1:A:234:VAL:O	1:A:235:LYS:C	2.58	0.41
1:A:55:ARG:HH22	1:A:57:GLU:HG3	1.87	0.40
1:A:121:LYS:HD2	1:A:158:THR:HA	2.03	0.40
1:A:156:TYR:N	1:A:156:TYR:CD1	2.89	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	306/316 (97%)	263 (86%)	32 (10%)	11 (4%)	3 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	SER
1	A	197	PRO
1	A	201	ALA
1	A	205	ARG
1	A	248	GLN
1	A	198	ARG
1	A	29	GLU
1	A	183	ARG
1	A	194	LEU
1	A	85	ASN
1	A	79	ILE

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	269/280 (96%)	218 (81%)	51 (19%)	1 4

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	6	LEU
1	A	8	ASP
1	A	12	THR
1	A	19	GLN
1	A	28	LEU
1	A	35	VAL
1	A	41	LEU
1	A	45	LYS
1	A	46	LYS
1	A	51	ASN
1	A	53	LEU
1	A	55	ARG
1	A	57	GLU

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Mol	Chain	Res	Type
1	A	58	VAL
1	A	59	LYS
1	A	64	ASN
1	A	71	LEU
1	A	77	LEU
1	A	80	GLN
1	A	84	GLU
1	A	85	ASN
1	A	98	LEU
1	A	107	GLN
1	A	113	HIS
1	A	115	GLN
1	A	119	LYS
1	A	122	THR
1	A	131	GLU
1	A	136	THR
1	A	141	GLU
1	A	159	LEU
1	A	177	ILE
1	A	187	LEU
1	A	192	LYS
1	A	193	SER
1	A	195	LYS
1	A	199	SER
1	A	200	VAL
1	A	205	ARG
1	A	214	ARG
1	A	222	LEU
1	A	230	ILE
1	A	245	LYS
1	A	248	GLN
1	A	265	ARG
1	A	292	GLN
1	A	299	ILE
1	A	305	LEU
1	A	307	VAL
1	A	309	ASP

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

Mol	Chain	Res	Type
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	19	GLN
1	A	27	HIS
1	A	30	GLN
1	A	50	HIS
1	A	51	ASN
1	A	60	GLN
1	A	67	GLN
1	A	73	HIS
1	A	76	HIS
1	A	80	GLN
1	A	81	GLN
1	A	85	ASN
1	A	113	HIS
1	A	144	HIS
1	A	180	ASN
1	A	209	GLN
1	A	217	GLN
1	A	237	GLN
1	A	248	GLN
1	A	250	GLN
1	A	279	ASN
1	A	294	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are 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	$\#\|Z\| > 2$
5	MPD	B	401	-	7,7,7	1.62	2 (28%)	9,10,10	1.86	4 (44%)

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
5	MPD	B	401	-	-	1/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	MPD	C1-C2	2.99	1.61	1.52
5	B	401	MPD	C3-C2	2.12	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	401	MPD	O4-C4-C3	-2.99	99.27	111.36
5	B	401	MPD	O2-C2-C3	-2.70	99.65	109.80
5	B	401	MPD	C1-C2-C3	2.13	119.87	109.96
5	B	401	MPD	CM-C2-C1	2.11	114.97	110.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	MPD	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	MPD	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 (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	308/316 (97%)	-0.36	5 (1%) 72 66	24, 41, 85, 135	0
2	B	15/16 (93%)	-0.43	0 100 100	31, 42, 112, 136	0
3	C	15/16 (93%)	-0.34	0 100 100	30, 43, 108, 130	0
All	All	338/348 (97%)	-0.36	5 (1%) 73 68	24, 42, 92, 136	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	SER	3.2
1	A	201	ALA	2.8
1	A	198	ARG	2.2
1	A	197	PRO	2.1
1	A	84	GLU	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 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, 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
5	MPD	B	401	8/8	0.83	0.22	29,32,35,37	0
4	IOD	A	1005	1/1	0.92	0.09	84,84,84,84	1
4	IOD	A	1004	1/1	0.97	0.14	62,62,62,62	1
4	IOD	A	1003	1/1	0.99	0.09	55,55,55,55	1
4	IOD	A	1002	1/1	0.99	0.10	52,52,52,52	1
4	IOD	A	1001	1/1	1.00	0.09	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.