Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2018 – 09:06 PM EST

PDB ID	:	3ER9
Title	:	Crystal structure of the heterodimeric vaccinia virus mRNA polyadenylate polymerase complex with UU and 3'-deoxy ATP
Authors	:	Li, C.; Li, H.; Zhou, S.; Poulos, T.L.; Gershon, P.D.
Deposited on	:	2008-10-01
Resolution	:	2.06 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736
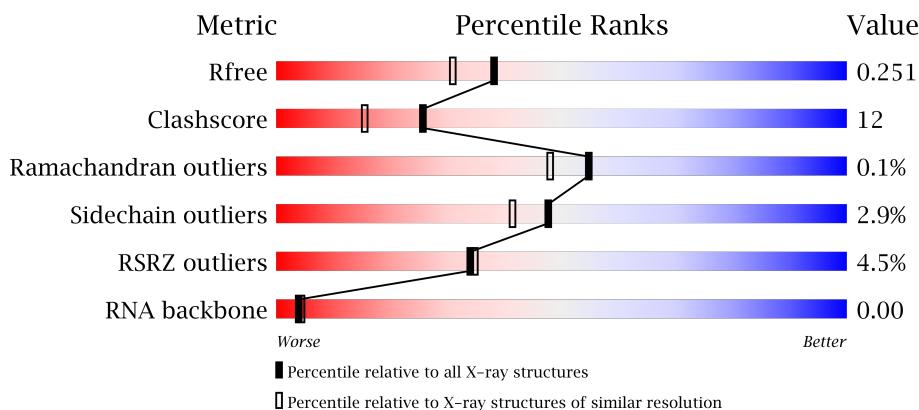
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
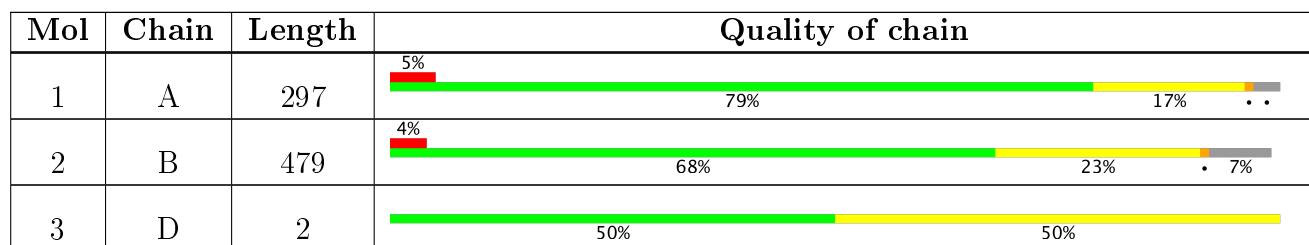
The reported resolution of this entry is 2.06 Å.

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}	100719	2028 (2.08-2.04)
Clashscore	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)
RSRZ outliers	101464	2035 (2.08-2.04)
RNA backbone	2435	1078 (2.70-1.42)

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 <=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	297	5% 79% 17% · ·
2	B	479	4% 68% 23% · 7%
3	D	2	50% 50%

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	GOL	A	880	-		-	X
4	GOL	A	890	-		-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6416 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 Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2382	1552	394	424	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	ARG	ENGINEERED	UNP P07617
A	142	ALA	LYS	ENGINEERED	UNP P07617
A	143	ALA	ARG	ENGINEERED	UNP P07617

- Molecule 2 is a protein called Poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	445	Total	C	N	O	S	0	0	0
			3627	2318	605	680	24			
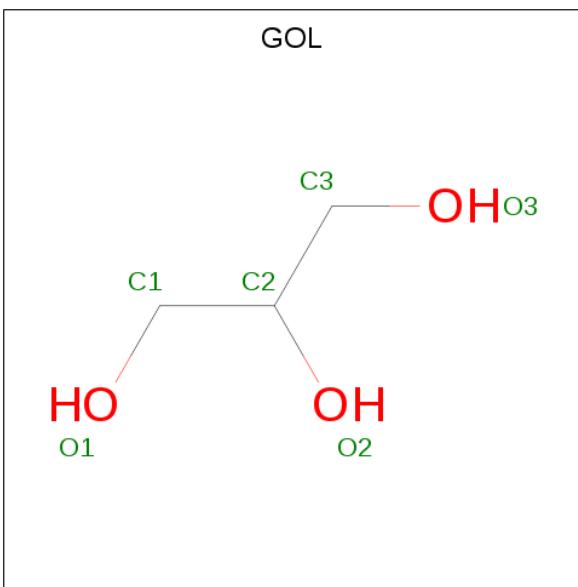
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	SER	LEU	ENGINEERED	UNP P23371

- Molecule 3 is a RNA chain called 5'-R(UP*U)-3'.
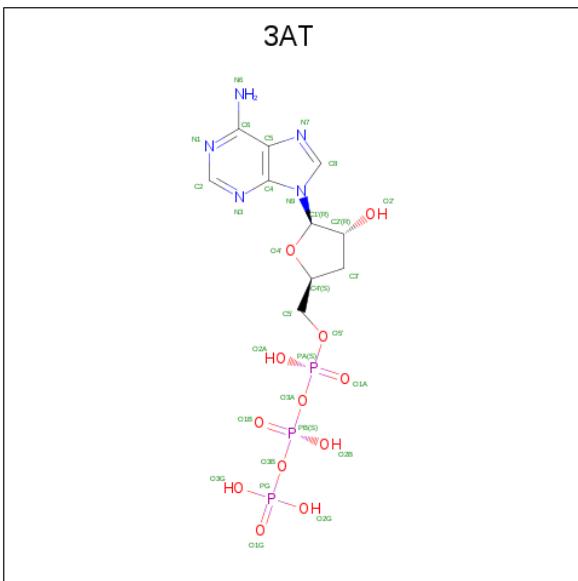
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	P	0	0	0
			40	18	4	16	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 5 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

3AT

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	Ca 2	0	0
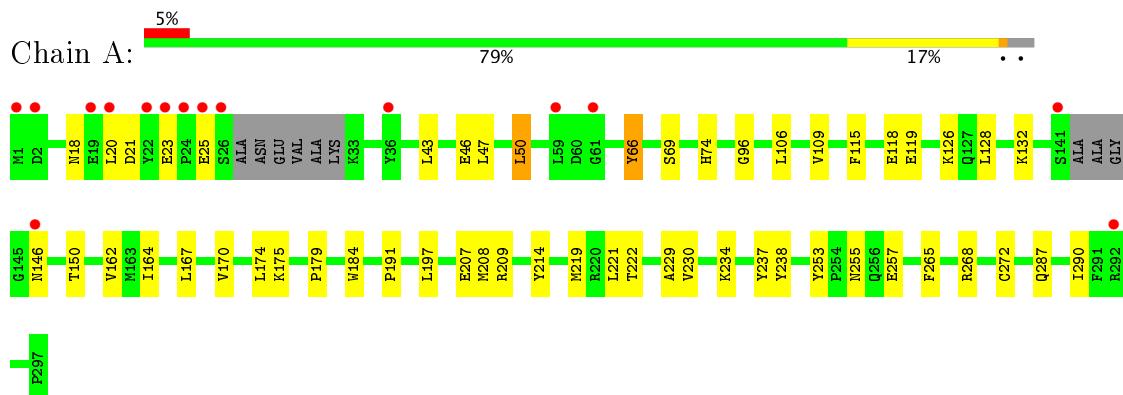
- Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total 135	O 135	0	0
7	B	182	Total 182	O 182	0	0
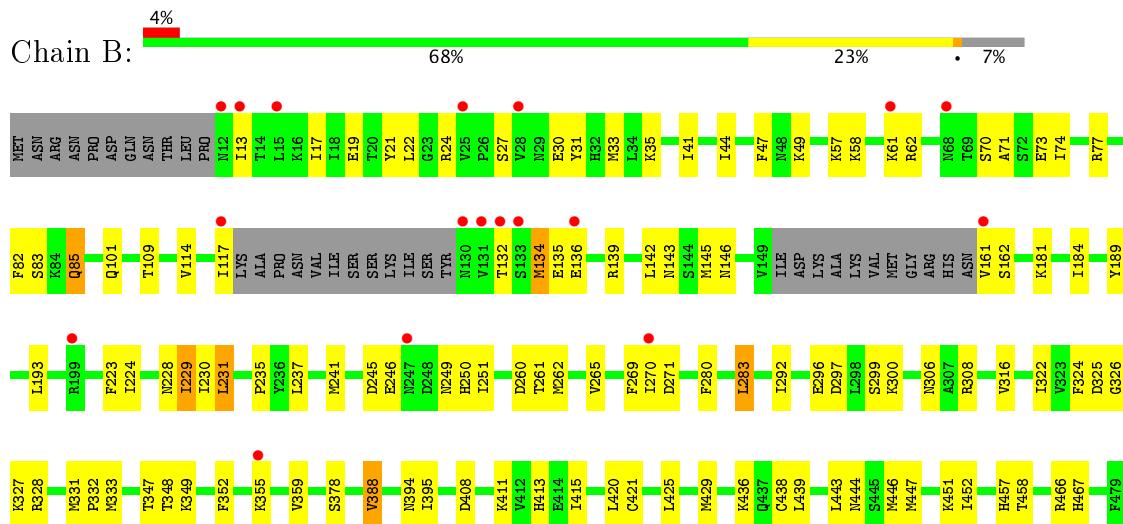
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
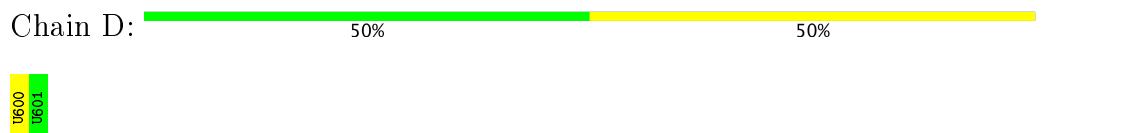
- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase

- Molecule 2: Poly(A) polymerase catalytic subunit

- Molecule 3: 5'-R(UP*U)-3'

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.53Å 91.98Å 133.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.69 – 2.06 42.69 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.1 (42.69-2.06) 97.8 (42.69-2.06)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	0.53	Depositor
$<I/\sigma(I)>$ [1]	1.46 (at 2.05Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.250 0.208 , 0.251	Depositor DCC
R_{free} test set	2660 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.5	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6416	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, CA, 3AT

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	0.40	0/2444	0.65	0/3308
2	B	0.35	0/3686	0.59	0/4972
3	D	0.78	0/43	1.22	0/64
All	All	0.38	0/6173	0.62	0/8344

There are no bond length outliers.

There are no bond angle outliers.

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	2382	0	2389	29	0
2	B	3627	0	3689	114	0
3	D	40	0	21	2	0
4	A	18	0	24	2	0
5	B	30	0	12	0	0
6	B	2	0	0	0	0
7	A	135	0	0	3	0
7	B	182	0	0	7	0
All	All	6416	0	6135	145	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 12.

All (145) 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:B:444:ASN:HA	2:B:447:MET:HE3	1.38	1.01
2:B:413:HIS:HD2	2:B:415:ILE:H	1.13	0.96
2:B:283:LEU:HD22	2:B:429:MET:HE1	1.52	0.90
2:B:280:PHE:HA	2:B:429:MET:HE3	1.53	0.89
2:B:21:TYR:CZ	2:B:85:GLN:HG2	2.11	0.86
2:B:283:LEU:HD22	2:B:429:MET:CE	2.10	0.82
2:B:61:LYS:HZ3	2:B:62:ARG:HG3	1.44	0.81
2:B:184:ILE:HG21	2:B:262:MET:HE1	1.64	0.80
2:B:280:PHE:HA	2:B:429:MET:CE	2.16	0.75
2:B:70:SER:OG	2:B:73:GLU:HG3	1.86	0.75
2:B:85:GLN:HB2	7:B:1221:HOH:O	1.86	0.74
2:B:331:MET:HE3	2:B:421:CYS:HB3	1.70	0.73
2:B:316:VAL:CG1	2:B:322:ILE:HD12	2.18	0.72
2:B:331:MET:HG3	2:B:332:PRO:HA	1.70	0.72
2:B:74:ILE:HD12	2:B:224:ILE:HA	1.71	0.72
2:B:413:HIS:CD2	2:B:415:ILE:H	2.05	0.71
1:A:118:GLU:HG2	1:A:162:VAL:HG11	1.73	0.69
2:B:328:ARG:HG2	2:B:331:MET:O	1.91	0.69
2:B:408:ASP:HB2	2:B:411:LYS:HD2	1.74	0.69
2:B:61:LYS:NZ	2:B:62:ARG:HG3	2.08	0.68
1:A:164:ILE:HD11	1:A:174:LEU:HD11	1.73	0.68
2:B:22:LEU:HA	7:B:1221:HOH:O	1.96	0.66
2:B:327:LYS:HG3	2:B:327:LYS:O	1.96	0.65
2:B:235:PRO:HG3	2:B:466:ARG:O	1.96	0.65
1:A:23:GLU:HB3	1:A:25:GLU:OE1	1.97	0.65
2:B:324:PHE:HA	2:B:444:ASN:HD21	1.62	0.63
2:B:146:ASN:HD21	2:B:299:SER:HA	1.63	0.63
2:B:27:SER:OG	2:B:30:GLU:HG3	1.98	0.63
1:A:66:TYR:CD1	1:A:69:SER:HB3	2.34	0.63
2:B:280:PHE:CD1	2:B:429:MET:HE3	2.33	0.63
2:B:297:ASP:HA	2:B:300:LYS:HE3	1.80	0.63
2:B:231:LEU:HD13	2:B:241:MET:HE2	1.81	0.62
2:B:132:THR:HA	2:B:135:GLU:OE2	1.97	0.62
2:B:143:ASN:O	2:B:451:LYS:HE2	2.00	0.62
2:B:142:LEU:HA	2:B:145:MET:HE3	1.82	0.62
2:B:326:GLY:H	2:B:444:ASN:HD22	1.46	0.62
2:B:325:ASP:OD2	2:B:327:LYS:HG2	1.99	0.61
4:A:890:GOL:H32	7:A:1204:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:HIS:HE1	2:B:452:ILE:O	1.86	0.59
2:B:378:SER:HB3	2:B:388:VAL:HG13	1.85	0.59
2:B:13:ILE:O	2:B:17:ILE:HG12	2.02	0.59
2:B:58:LYS:O	2:B:61:LYS:HG3	2.02	0.59
2:B:261:THR:O	2:B:265:VAL:HG23	2.02	0.58
2:B:316:VAL:HG11	2:B:322:ILE:HD12	1.84	0.58
1:A:253:TYR:OH	1:A:287:GLN:NE2	2.36	0.58
2:B:61:LYS:HD2	2:B:62:ARG:N	2.19	0.58
2:B:22:LEU:HD23	7:B:1221:HOH:O	2.03	0.57
2:B:139:ARG:HG2	2:B:306:ASN:ND2	2.20	0.57
2:B:21:TYR:OH	2:B:85:GLN:HG2	2.03	0.57
1:A:265:PHE:HA	1:A:268:ARG:HD3	1.85	0.56
2:B:230:ILE:N	2:B:230:ILE:HD12	2.20	0.56
2:B:74:ILE:CD1	2:B:224:ILE:HA	2.35	0.56
2:B:245:ASP:OD1	2:B:249:ASN:HB2	2.05	0.56
2:B:142:LEU:HD23	2:B:145:MET:HE3	1.87	0.56
2:B:189:TYR:CE2	2:B:193:LEU:HD21	2.40	0.56
2:B:326:GLY:H	2:B:444:ASN:ND2	2.03	0.55
2:B:161:VAL:N	2:B:250:HIS:HB3	2.22	0.55
2:B:82:PHE:C	2:B:85:GLN:HE22	2.09	0.55
2:B:443:LEU:HD23	2:B:446:MET:HE1	1.88	0.55
2:B:184:ILE:HD13	2:B:262:MET:CE	2.35	0.55
2:B:280:PHE:CA	2:B:429:MET:HE3	2.32	0.55
1:A:20:LEU:HD22	1:A:237:TYR:CE2	2.42	0.54
2:B:280:PHE:HD1	2:B:429:MET:HE3	1.72	0.54
1:A:255:ASN:OD1	1:A:257:GLU:OE1	2.25	0.54
2:B:162:SER:OG	2:B:251:ILE:HD13	2.08	0.54
2:B:229:ILE:N	2:B:229:ILE:HD13	2.24	0.53
2:B:355:LYS:HE2	7:B:1264:HOH:O	2.07	0.53
2:B:31:TYR:O	2:B:35:LYS:HB2	2.08	0.53
2:B:57:LYS:HE2	2:B:71:ALA:HB1	1.90	0.52
2:B:331:MET:CG	2:B:332:PRO:HA	2.38	0.52
2:B:348:THR:HB	2:B:352:PHE:HD1	1.74	0.52
1:A:132:LYS:HG3	1:A:170:VAL:HG11	1.91	0.52
2:B:283:LEU:CD2	2:B:429:MET:CE	2.87	0.51
2:B:109:THR:O	2:B:114:VAL:HG23	2.11	0.51
2:B:85:GLN:CD	2:B:85:GLN:H	2.14	0.51
1:A:230:VAL:HG13	1:A:234:LYS:HE2	1.93	0.51
2:B:33:MET:HA	2:B:33:MET:CE	2.41	0.51
2:B:228:ASN:HB2	2:B:246:GLU:HG2	1.93	0.50
2:B:184:ILE:HD13	2:B:262:MET:HE1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:PHE:O	2:B:49:LYS:HE3	2.12	0.50
1:A:20:LEU:HD22	1:A:237:TYR:CD2	2.46	0.50
2:B:85:GLN:H	2:B:85:GLN:NE2	2.09	0.50
2:B:189:TYR:O	2:B:193:LEU:CD2	2.58	0.50
2:B:189:TYR:O	2:B:193:LEU:HD23	2.11	0.50
2:B:33:MET:HE2	2:B:33:MET:HA	1.94	0.50
2:B:49:LYS:HD2	2:B:82:PHE:CG	2.47	0.50
2:B:83:SER:N	2:B:85:GLN:HE22	2.08	0.50
2:B:139:ARG:O	2:B:143:ASN:ND2	2.45	0.49
2:B:229:ILE:HD13	2:B:229:ILE:H	1.76	0.49
2:B:117:ILE:HG23	3:D:600:U:C4	2.48	0.49
2:B:229:ILE:C	2:B:230:ILE:HD12	2.33	0.49
2:B:117:ILE:HG23	3:D:600:U:O4	2.14	0.48
2:B:229:ILE:H	2:B:229:ILE:CD1	2.26	0.48
2:B:136:GLU:HG2	7:B:1272:HOH:O	2.13	0.48
1:A:96:GLY:HA3	1:A:115:PHE:CE1	2.48	0.47
1:A:126:LYS:HB2	1:A:126:LYS:NZ	2.30	0.47
4:A:880:GOL:H31	7:A:1306:HOH:O	2.15	0.46
2:B:260:ASP:OD1	2:B:261:THR:N	2.48	0.46
2:B:283:LEU:CD2	2:B:429:MET:HE2	2.45	0.46
2:B:230:ILE:HD11	7:B:1110:HOH:O	2.15	0.46
2:B:142:LEU:HD23	2:B:145:MET:CE	2.45	0.46
2:B:297:ASP:HA	2:B:300:LYS:CE	2.45	0.46
1:A:230:VAL:CG1	1:A:234:LYS:HE2	2.45	0.46
2:B:58:LYS:CG	2:B:61:LYS:HZ1	2.28	0.46
2:B:408:ASP:HB2	2:B:411:LYS:CD	2.43	0.46
1:A:106:LEU:HB2	1:A:109:VAL:HG13	1.98	0.45
2:B:269:PHE:O	2:B:270:ILE:HD13	2.17	0.45
2:B:283:LEU:HD22	2:B:429:MET:HE2	1.96	0.45
2:B:457:HIS:HD2	2:B:458:THR:O	1.99	0.45
2:B:134:MET:HA	2:B:134:MET:CE	2.47	0.45
1:A:219:MET:HE2	1:A:221:LEU:HD21	1.98	0.44
2:B:331:MET:CE	2:B:438:CYS:SG	3.06	0.44
2:B:58:LYS:HG2	2:B:61:LYS:NZ	2.32	0.44
1:A:184:TRP:CZ3	1:A:229:ALA:HB2	2.53	0.44
2:B:58:LYS:HG2	2:B:61:LYS:HZ1	1.82	0.44
2:B:83:SER:CA	2:B:85:GLN:HE22	2.30	0.44
1:A:272:CYS:SG	7:A:1313:HOH:O	2.62	0.44
2:B:193:LEU:HD12	2:B:271:ASP:OD1	2.18	0.44
2:B:57:LYS:CE	2:B:71:ALA:HB1	2.47	0.44
1:A:119:GLU:HA	1:A:119:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:OE1	1:A:74:HIS:NE2	2.50	0.43
2:B:74:ILE:HD13	2:B:77:ARG:NH1	2.34	0.43
2:B:296:GLU:O	2:B:300:LYS:HE2	2.18	0.43
2:B:394:ASN:O	2:B:395:ILE:HD13	2.19	0.43
2:B:283:LEU:HD21	2:B:425:LEU:HB3	2.00	0.43
2:B:467:HIS:HE1	7:B:1130:HOH:O	2.01	0.43
2:B:44:ILE:HD13	2:B:101:GLN:HE21	1.83	0.43
2:B:308:ARG:HG3	2:B:308:ARG:HH11	1.84	0.42
1:A:43:LEU:HD13	1:A:290:ILE:HG23	2.01	0.42
2:B:444:ASN:ND2	2:B:447:MET:HE1	2.34	0.42
2:B:19:GLU:HG3	2:B:24:ARG:O	2.19	0.42
2:B:77:ARG:HD2	2:B:223:PHE:O	2.20	0.42
2:B:324:PHE:HB3	2:B:447:MET:HE1	2.01	0.42
1:A:164:ILE:CD1	1:A:191:PRO:HG2	2.50	0.41
1:A:175:LYS:HE2	1:A:207:GLU:OE2	2.20	0.41
1:A:150:THR:HG23	1:A:179:PRO:HB3	2.02	0.41
2:B:359:VAL:HG11	2:B:420:LEU:CD2	2.51	0.41
2:B:21:TYR:CG	2:B:41:ILE:HG23	2.55	0.41
1:A:18:ASN:HB3	1:A:238:TYR:CE2	2.56	0.41
1:A:46:GLU:O	1:A:50:LEU:HB2	2.20	0.41
1:A:164:ILE:HD13	1:A:214:TYR:OH	2.20	0.41
2:B:333:MET:HB3	2:B:347:THR:O	2.21	0.41
2:B:283:LEU:CD1	2:B:439:LEU:HD13	2.51	0.40
1:A:20:LEU:HD23	1:A:21:ASP:N	2.36	0.40
1:A:25:GLU:H	1:A:25:GLU:CD	2.25	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	282/297 (95%)	275 (98%)	6 (2%)	1 (0%)	38	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	439/479 (92%)	426 (97%)	13 (3%)	0	100	100
All	All	721/776 (93%)	701 (97%)	19 (3%)	1 (0%)	55	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASN

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	266/270 (98%)	257 (97%)	9 (3%)	42	35
2	B	422/453 (93%)	411 (97%)	11 (3%)	51	46
All	All	688/723 (95%)	668 (97%)	20 (3%)	48	41

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	50	LEU
1	A	66	TYR
1	A	128	LEU
1	A	167	LEU
1	A	197	LEU
1	A	208	MET
1	A	209	ARG
1	A	222	THR
2	B	85	GLN
2	B	134	MET
2	B	181	LYS
2	B	229	ILE
2	B	231	LEU
2	B	237	LEU

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Mol	Chain	Res	Type
2	B	283	LEU
2	B	292	ILE
2	B	349	LYS
2	B	388	VAL
2	B	436	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	156	ASN
1	A	231	ASN
1	A	287	GLN
1	A	288	GLN
2	B	32	HIS
2	B	59	ASN
2	B	85	GLN
2	B	101	GLN
2	B	143	ASN
2	B	180	ASN
2	B	247	ASN
2	B	306	ASN
2	B	329	ASN
2	B	413	HIS
2	B	428	GLN
2	B	444	ASN
2	B	457	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	GOL	A	880	-	5,5,5	0.52	0	5,5,5	0.31	0
4	GOL	A	890	-	5,5,5	0.54	0	5,5,5	0.35	0
4	GOL	A	900	-	5,5,5	0.50	0	5,5,5	0.33	0
5	3AT	B	800	6	26,32,32	1.39	5 (19%)	21,50,50	2.82	4 (19%)

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
4	GOL	A	880	-	-	0/4/4/4	0/0/0/0
4	GOL	A	890	-	-	0/4/4/4	0/0/0/0
4	GOL	A	900	-	-	0/4/4/4	0/0/0/0
5	3AT	B	800	6	-	0/18/34/34	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800	3AT	C8-N7	-2.60	1.29	1.34
5	B	800	3AT	C2-N3	2.21	1.35	1.32
5	B	800	3AT	C2'-C1'	2.28	1.56	1.53
5	B	800	3AT	C5-C4	2.30	1.45	1.40
5	B	800	3AT	PG-O1G	2.66	1.59	1.50

All (4) bond angle outliers are listed below:

Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	800	3AT	N3-C2-N1	-11.40	118.93	128.86
5	B	800	3AT	C3'-C4'-C5'	-2.70	109.11	113.81
5	B	800	3AT	C2-N1-C6	2.69	123.48	118.77
5	B	800	3AT	O4'-C4'-C3'	3.31	109.39	105.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	880	GOL	1	0
4	A	890	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 (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	288/297 (96%)	0.20	15 (5%)	28	28	17, 28, 50, 82	0
2	B	445/479 (92%)	0.31	18 (4%)	39	41	19, 34, 54, 85	0
3	D	2/2 (100%)	0.15	0	100	100	47, 47, 47, 59	0
All	All	735/778 (94%)	0.27	33 (4%)	34	35	17, 31, 54, 85	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
2	B	161	VAL	5.9
2	B	132	THR	5.6
1	A	24	PRO	5.4
2	B	130	ASN	5.2
2	B	199	ARG	4.3
1	A	20	LEU	4.1
1	A	25	GLU	4.0
1	A	146	ASN	4.0
2	B	117	ILE	3.8
2	B	133	SER	3.8
2	B	15	LEU	3.7
1	A	23	GLU	3.7
1	A	141	SER	3.2
2	B	131	VAL	3.2
2	B	28	VAL	3.2
2	B	61	LYS	3.0
2	B	13	ILE	3.0
1	A	292	ARG	2.8
2	B	25	VAL	2.7
1	A	19	GLU	2.7
2	B	136	GLU	2.6
2	B	12	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	SER	2.4
2	B	68	ASN	2.3
1	A	22	TYR	2.3
1	A	2	ASP	2.3
1	A	36	TYR	2.2
1	A	61	GLY	2.2
2	B	247	ASN	2.1
1	A	59	LEU	2.0
2	B	270	ILE	2.0
2	B	355	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	A	880	6/6	0.86	0.25	16.83	57,58,59,62	0
4	GOL	A	890	6/6	0.72	0.26	11.90	61,63,65,68	0
5	3AT	B	800	30/30	0.96	0.12	-0.26	28,35,38,41	0
4	GOL	A	900	6/6	0.82	0.20	-	65,66,66,67	0
6	CA	B	901	1/1	0.96	0.06	-	33,33,33,33	0
6	CA	B	902	1/1	0.85	0.09	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.