



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 01:12 AM EDT

PDB ID : 5L1Z  
Title : TAR complex with HIV-1 Tat-AFF4-P-TEFb  
Authors : Schulze-Gahmen, U.; Hurley, J.  
Deposited on : 2016-07-29  
Resolution : 5.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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

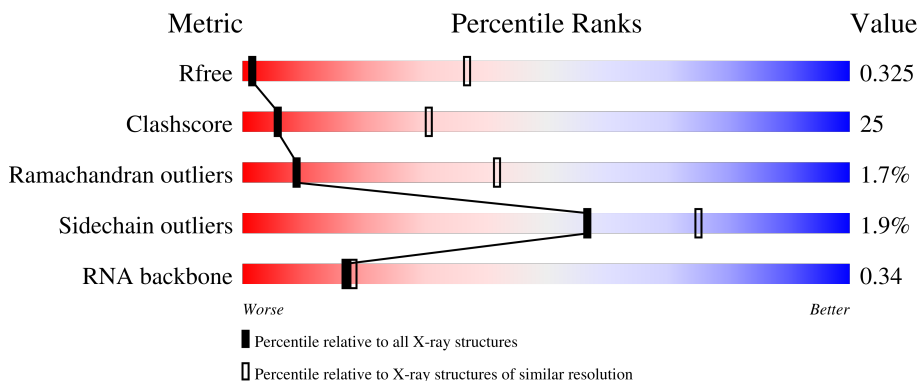
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.90 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	1016 (7.94-3.86)
Clashscore	141614	1042 (7.88-3.90)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)
RNA backbone	3102	1076 (8.70-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	330	
2	B	264	
3	C	36	
4	D	58	
5	N	23	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5713 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 Cyclin-dependent kinase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	311	2515	1611	434	454	1	15	0	0	0

- Molecule 2 is a protein called Cyclin-T1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	255	2085	1333	362	380	10	0	0	0

- Molecule 3 is a protein called AF4/FMR2 family member 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	34	276	175	43	56	2	0	0	0

- Molecule 4 is a protein called Protein Tat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	50	388	246	68	66	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ACE	-	acetylation	UNP P69697

- Molecule 5 is a RNA chain called RNA (5'-R(P\*AP\*GP\*AP\*UP\*CP\*UP\*GP\*AP\*GP\*CP\*CP\*UP\*GP\*GP\*GP\*AP\*GP\*CP\*UP\*CP\*UP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	N	21	447	199	78	149	21	0	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	Zn 2	0	0



- Molecule 4: Protein Tat

Chain D:  34% 48% 14%



- Molecule 5: RNA (5'-R(P\*AP\*GP\*AP\*UP\*CP\*UP\*GP\*AP\*GP\*CP\*CP\*UP\*GP\*GP\*GP\*A P\*GP\*CP\*UP\*CP\*UP\*CP\*U)-3')

Chain N:  17% 57% 17% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.87Å 146.87Å 103.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 5.90 48.07 – 5.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (500.00-5.90) 100.0 (48.07-5.90)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 5.73Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.313 0.237 , 0.325	Depositor DCC
$R_{free}$ test set	347 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	360.9	Xtrriage
Anisotropy	0.463	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 380.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.105 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5713	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	424.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, ACE, ZN

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	0.23	0/2552	0.44	0/3440
2	B	0.24	0/2139	0.45	0/2915
3	C	0.29	0/280	0.47	0/371
4	D	0.25	0/398	0.43	0/538
5	N	0.27	0/498	0.66	0/774
All	All	0.24	0/5867	0.47	0/8038

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	2515	0	2572	106	1
2	B	2085	0	2060	118	0
3	C	276	0	271	35	0
4	D	388	0	377	47	0
5	N	447	0	227	23	1
6	D	2	0	0	0	0
All	All	5713	0	5507	284	2

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 (284) 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)
4:D:49:ARG:NE	4:D:49:ARG:H	1.69	0.90
2:B:248:THR:HG21	4:D:43:LEU:HD22	1.53	0.89
4:D:25:CYS:C	5:N:33:G:H22	1.78	0.87
1:A:268:VAL:HG21	1:A:271:GLN:HG2	1.58	0.84
2:B:251:ARG:H	2:B:251:ARG:HD3	1.43	0.83
1:A:181:GLN:H	1:A:181:GLN:NE2	1.77	0.81
2:B:158:VAL:HG12	2:B:162:GLN:HE21	1.46	0.81
2:B:250:ASN:CG	4:D:44:GLY:HA3	2.03	0.79
3:C:47:LYS:NZ	3:C:47:LYS:HA	1.99	0.78
2:B:25:ARG:NH2	2:B:31:PRO:HA	2.01	0.76
2:B:56:GLN:HG3	2:B:60:ASN:HD21	1.53	0.74
2:B:185:THR:HG22	2:B:244:ILE:HD12	1.70	0.73
2:B:203:LEU:HD13	2:B:238:THR:HG23	1.70	0.73
3:C:44:LYS:N	3:C:44:LYS:HE3	2.05	0.71
2:B:10:LYS:NZ	2:B:10:LYS:HA	2.05	0.70
4:D:25:CYS:HA	5:N:33:G:H1	1.55	0.70
2:B:67:HIS:HB3	2:B:189:LEU:HD11	1.74	0.69
2:B:84:ALA:HB3	2:B:85:PRO:HD3	1.75	0.69
2:B:155:THR:HG23	4:D:6:PRO:HB3	1.74	0.68
2:B:177:MET:HA	2:B:180:ASN:HD22	1.58	0.67
1:A:196:PRO:HD2	1:A:199:LEU:HD12	1.77	0.67
3:C:63:LYS:HA	3:C:63:LYS:HE3	1.77	0.67
3:C:58:ASN:HD22	3:C:61:GLU:HG3	1.59	0.67
2:B:148:LEU:O	2:B:150:ILE:HG12	1.96	0.66
1:A:73:LEU:HD13	1:A:140:ILE:HG22	1.77	0.65
5:N:29:C:H2'	5:N:30:C:C6	2.31	0.65
2:B:163:LEU:HG	3:C:35:PHE:HD2	1.60	0.65
3:C:62:MET:HG2	4:D:28:LYS:NZ	2.11	0.65
1:A:187:ASN:HD21	1:A:202:GLY:HA2	1.62	0.64
2:B:83:VAL:HA	2:B:136:LEU:HD21	1.78	0.64
1:A:186:TPO:P	1:A:186:TPO:H	2.19	0.64
5:N:26:G:O2'	5:N:27:A:H5'	1.98	0.64
2:B:168:LYS:NZ	2:B:168:LYS:HB3	2.12	0.64
5:N:33:G:H5''	5:N:34:G:N3	2.13	0.63
2:B:254:ARG:HE	2:B:254:ARG:HA	1.63	0.63
4:D:26:TYR:N	5:N:33:G:H22	1.97	0.63
2:B:94:VAL:HG22	2:B:148:LEU:HD13	1.80	0.62
2:B:175:TYR:CD2	4:D:3:PRO:HA	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LYS:HA	2:B:10:LYS:HZ1	1.63	0.62
2:B:55:SER:HB3	2:B:97:GLN:HE22	1.62	0.62
2:B:57:LEU:HD22	4:D:13:HIS:CE1	2.35	0.62
3:C:65:PHE:CZ	4:D:29:LYS:HG2	2.35	0.62
2:B:96:GLU:HG3	4:D:11:TRP:HE3	1.64	0.61
4:D:49:ARG:NE	4:D:49:ARG:N	2.46	0.61
2:B:203:LEU:HD11	2:B:242:LEU:HD21	1.82	0.61
2:B:213:PRO:HG3	3:C:39:TYR:CE2	2.36	0.61
1:A:207:GLY:O	1:A:210:ILE:HG12	2.00	0.61
2:B:164:VAL:O	3:C:38:PRO:HD3	2.01	0.60
5:N:33:G:H3'	5:N:34:G:H5'	1.83	0.60
2:B:226:ASP:HB3	2:B:229:VAL:HG23	1.82	0.60
1:A:10:CYS:SG	1:A:13:CYS:HB3	2.42	0.60
1:A:25:ILE:HD11	1:A:35:LYS:HB2	1.83	0.60
2:B:56:GLN:HG3	2:B:60:ASN:ND2	2.17	0.59
1:A:196:PRO:HB2	1:A:198:GLU:OE1	2.02	0.59
4:D:40:THR:O	4:D:44:GLY:HA2	2.03	0.59
1:A:175:SER:HB2	4:D:9:GLU:HG3	1.85	0.59
3:C:48:LEU:O	3:C:52:ILE:HG13	2.03	0.59
3:C:62:MET:HG2	4:D:28:LYS:HZ3	1.66	0.58
1:A:213:TRP:HB2	1:A:303:ARG:NH1	2.18	0.58
1:A:163:LEU:HD23	1:A:164:LYS:N	2.18	0.58
2:B:67:HIS:O	2:B:71:MET:HG2	2.03	0.57
1:A:214:GLY:O	1:A:218:ILE:HG13	2.04	0.57
4:D:2:GLU:OE2	4:D:3:PRO:HD2	2.04	0.57
5:N:27:A:H2'	5:N:28:G:H8	1.69	0.57
1:A:151:LYS:HE3	1:A:153:ALA:HB3	1.86	0.56
1:A:80:ASN:HB3	1:A:104:ASP:OD2	2.05	0.56
2:B:155:THR:HA	4:D:6:PRO:CG	2.35	0.56
2:B:155:THR:HG23	4:D:6:PRO:CB	2.36	0.56
5:N:27:A:H2'	5:N:28:G:C8	2.40	0.56
1:A:151:LYS:HE2	1:A:154:ASN:HD21	1.70	0.56
3:C:47:LYS:HA	3:C:47:LYS:HZ1	1.69	0.56
4:D:11:TRP:HE1	4:D:12:LYS:HE2	1.71	0.55
2:B:166:ALA:HB1	2:B:170:LEU:HD23	1.88	0.55
1:A:278:ARG:HA	1:A:278:ARG:NE	2.20	0.55
1:A:52:MET:CE	1:A:98:SER:HA	2.36	0.55
1:A:278:ARG:HA	1:A:278:ARG:HE	1.71	0.55
1:A:224:THR:HG22	1:A:282:TYR:CD2	2.41	0.55
1:A:134:LEU:HB2	1:A:310:LEU:HD21	1.89	0.55
2:B:106:LYS:HG3	2:B:118:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:LEU:HB3	3:C:55:MET:O	2.07	0.54
1:A:187:ASN:ND2	1:A:202:GLY:HA2	2.21	0.54
2:B:101:LEU:HD21	2:B:130:VAL:HG13	1.88	0.54
2:B:155:THR:HA	4:D:6:PRO:HG3	1.89	0.54
2:B:250:ASN:OD1	4:D:44:GLY:HA3	2.08	0.54
3:C:34:LEU:HD13	3:C:34:LEU:O	2.08	0.54
5:N:22:A:H3'	5:N:23:U:C6	2.43	0.54
5:N:28:G:H2'	5:N:29:C:O4'	2.07	0.54
2:B:153:PRO:O	2:B:157:VAL:HG23	2.07	0.54
1:A:221:GLU:HA	1:A:224:THR:OG1	2.08	0.54
2:B:61:THR:HG22	2:B:65:TYR:CE2	2.42	0.54
2:B:242:LEU:HD23	2:B:245:LEU:HD12	1.89	0.53
2:B:35:LEU:HD23	2:B:35:LEU:O	2.08	0.53
2:B:59:ILE:O	2:B:63:ILE:HG13	2.08	0.53
2:B:96:GLU:HG3	4:D:11:TRP:CE3	2.42	0.53
1:A:114:LEU:O	1:A:225:ARG:HD2	2.07	0.53
2:B:10:LYS:O	2:B:10:LYS:HG3	2.09	0.53
2:B:254:ARG:HA	2:B:254:ARG:NE	2.23	0.53
1:A:151:LYS:HG2	1:A:154:ASN:ND2	2.24	0.52
2:B:130:VAL:O	2:B:134:VAL:HG23	2.09	0.52
3:C:63:LYS:C	3:C:65:PHE:H	2.12	0.52
2:B:82:SER:O	2:B:85:PRO:HD2	2.10	0.52
2:B:211:GLU:HB2	3:C:41:VAL:CG2	2.40	0.52
1:A:186:TPO:P	1:A:186:TPO:N	2.83	0.52
2:B:64:VAL:HG21	2:B:150:ILE:HG21	1.91	0.52
2:B:233:LEU:O	2:B:237:LEU:HG	2.10	0.52
2:B:244:ILE:HA	2:B:247:LYS:HE2	1.92	0.51
2:B:90:LEU:HD11	2:B:141:LEU:HD21	1.92	0.51
2:B:118:LEU:HD12	2:B:118:LEU:H	1.75	0.51
2:B:255:ILE:O	4:D:28:LYS:HB2	2.10	0.51
4:D:39:ILE:HD13	4:D:43:LEU:HD12	1.91	0.51
2:B:44:LEU:HG	2:B:48:MET:CE	2.41	0.51
2:B:193:PRO:HB2	2:B:194:PRO:HD3	1.92	0.51
1:A:239:ALA:O	1:A:243:GLN:HG3	2.11	0.51
3:C:44:LYS:O	3:C:44:LYS:HG2	2.11	0.51
5:N:39:C:H2'	5:N:40:U:C5	2.46	0.51
1:A:82:ILE:HD12	1:A:102:VAL:HG12	1.92	0.50
1:A:88:LYS:HE2	1:A:88:LYS:C	2.31	0.50
2:B:168:LYS:HB3	2:B:168:LYS:HZ3	1.75	0.50
2:B:205:CYS:HB3	2:B:210:TRP:O	2.12	0.50
4:D:49:ARG:H	4:D:49:ARG:CD	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:HB3	1:A:258:ASN:HD22	1.75	0.50
2:B:179:THR:OG1	4:D:0:ACE:H3	2.11	0.50
3:C:59:TYR:CD2	3:C:63:LYS:HD3	2.46	0.50
1:A:75:HIS:ND1	1:A:76:GLU:N	2.58	0.50
1:A:123:LEU:O	1:A:127:LYS:HG3	2.11	0.50
2:B:58:THR:HA	2:B:95:GLU:HG3	1.94	0.50
1:A:81:LEU:HD12	1:A:102:VAL:O	2.12	0.50
2:B:20:GLU:C	2:B:21:ASN:HD22	2.14	0.50
2:B:165:ARG:O	3:C:37:GLU:HG3	2.12	0.50
2:B:242:LEU:HD21	3:C:52:ILE:HG12	1.92	0.50
1:A:66:GLU:O	1:A:70:LEU:HG	2.11	0.50
1:A:133:LEU:HD12	1:A:165:LEU:HD21	1.92	0.50
2:B:207:TRP:HB2	3:C:52:ILE:HG21	1.93	0.50
1:A:212:LEU:N	1:A:212:LEU:HD12	2.27	0.50
3:C:59:TYR:O	3:C:63:LYS:HD2	2.12	0.50
4:D:25:CYS:HB3	4:D:30:CYS:SG	2.51	0.50
1:A:255:ASN:HB3	1:A:258:ASN:ND2	2.27	0.49
2:B:118:LEU:HD12	2:B:118:LEU:N	2.27	0.49
2:B:211:GLU:HB3	3:C:39:TYR:CE1	2.47	0.49
5:N:39:C:H2'	5:N:40:U:C6	2.47	0.49
2:B:240:GLU:O	2:B:244:ILE:HG13	2.13	0.49
2:B:42:ALA:HB1	2:B:183:HIS:ND1	2.26	0.49
2:B:184:LEU:HD21	4:D:43:LEU:HD13	1.94	0.49
1:A:299:ASP:OD2	1:A:301:ALA:HB3	2.12	0.49
2:B:158:VAL:HG12	2:B:162:GLN:NE2	2.23	0.49
4:D:38:PHE:O	4:D:42:ALA:HB3	2.12	0.49
1:A:176:LEU:N	1:A:176:LEU:HD12	2.28	0.49
1:A:294:LYS:O	1:A:304:ILE:HG22	2.13	0.49
3:C:61:GLU:HB3	4:D:28:LYS:HZ2	1.77	0.49
1:A:229:MET:SD	1:A:241:ILE:HG12	2.53	0.49
1:A:253:TRP:CD1	1:A:256:VAL:HB	2.48	0.49
2:B:209:ASN:O	3:C:41:VAL:HG23	2.13	0.49
2:B:261:CYS:HA	4:D:25:CYS:SG	2.53	0.49
1:A:32:GLU:OE2	1:A:51:LEU:HD11	2.13	0.49
1:A:130:MET:CE	1:A:219:MET:HB2	2.43	0.49
2:B:24:SER:HA	2:B:74:SER:OG	2.13	0.49
1:A:237:GLN:O	1:A:241:ILE:HG13	2.12	0.48
2:B:157:VAL:O	2:B:161:THR:HG23	2.13	0.48
2:B:163:LEU:HG	3:C:35:PHE:CD2	2.45	0.48
1:A:67:ILE:O	1:A:71:GLN:HG3	2.14	0.48
4:D:39:ILE:HG22	4:D:45:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:ARG:HH21	2:B:260:ALA:H	1.62	0.48
1:A:228:ILE:HG13	1:A:229:MET:HG3	1.95	0.48
2:B:178:ALA:HA	2:B:200:CYS:SG	2.53	0.48
2:B:256:TRP:O	2:B:257:ASN:ND2	2.47	0.48
2:B:55:SER:CB	2:B:97:GLN:HE22	2.25	0.48
1:A:65:ARG:O	1:A:69:ILE:HG13	2.13	0.48
1:A:108:HIS:CD2	1:A:113:LEU:HD21	2.48	0.48
1:A:110:LEU:HD11	1:A:222:MET:SD	2.54	0.48
1:A:148:ARG:C	1:A:190:VAL:HG22	2.34	0.48
3:C:47:LYS:HA	3:C:47:LYS:HZ2	1.75	0.47
1:A:200:LEU:HB2	1:A:238:LEU:HD21	1.96	0.47
2:B:14:PHE:N	2:B:14:PHE:CD1	2.82	0.47
5:N:22:A:N1	5:N:26:G:N7	2.62	0.47
1:A:137:LEU:HD21	1:A:150:MET:CE	2.44	0.47
1:A:257:ASP:HA	1:A:262:TYR:CD2	2.50	0.47
2:B:23:PRO:HB2	2:B:73:GLN:O	2.15	0.47
2:B:118:LEU:H	2:B:118:LEU:CD1	2.28	0.47
3:C:63:LYS:HE3	3:C:63:LYS:CA	2.44	0.47
2:B:60:ASN:O	2:B:64:VAL:HG23	2.15	0.47
5:N:30:C:H1'	5:N:36:G:N2	2.30	0.47
5:N:35:A:H2'	5:N:36:G:H5'	1.97	0.47
1:A:163:LEU:HD23	1:A:163:LEU:C	2.36	0.46
1:A:180:SER:HB2	1:A:181:GLN:NE2	2.29	0.46
2:B:55:SER:HA	4:D:14:PRO:O	2.14	0.46
2:B:175:TYR:CB	4:D:3:PRO:HG3	2.46	0.46
2:B:232:GLU:H	2:B:232:GLU:CD	2.19	0.46
1:A:212:LEU:HD12	1:A:212:LEU:H	1.81	0.46
2:B:207:TRP:O	3:C:59:TYR:HB2	2.15	0.46
2:B:250:ASN:HB2	4:D:43:LEU:C	2.36	0.46
3:C:59:TYR:CG	3:C:63:LYS:HD3	2.51	0.46
4:D:35:GLN:O	4:D:39:ILE:HG12	2.15	0.46
1:A:327:MET:SD	1:A:327:MET:C	2.95	0.46
3:C:62:MET:O	3:C:63:LYS:HE3	2.16	0.46
1:A:195:ARG:HD2	1:A:200:LEU:HD21	1.98	0.45
1:A:151:LYS:HG2	1:A:154:ASN:HD22	1.82	0.45
1:A:253:TRP:CG	1:A:256:VAL:HB	2.51	0.45
2:B:136:LEU:O	2:B:140:ILE:HG13	2.15	0.45
2:B:248:THR:HA	2:B:249:PRO:HD3	1.78	0.45
1:A:122:THR:OG1	1:A:125:GLU:HG3	2.17	0.45
1:A:129:VAL:HG22	1:A:324:LEU:HD11	1.97	0.45
1:A:125:GLU:O	1:A:129:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:ARG:O	4:D:49:ARG:HG2	2.16	0.45
2:B:113:HIS:N	2:B:114:PRO:HD3	2.31	0.45
2:B:208:SER:HB2	2:B:210:TRP:HD1	1.82	0.45
1:A:151:LYS:HE2	1:A:154:ASN:ND2	2.32	0.45
2:B:49:GLY:O	2:B:54:VAL:HG22	2.17	0.45
2:B:131:GLN:O	2:B:135:ILE:HG13	2.17	0.44
1:A:130:MET:HE1	1:A:219:MET:HB2	2.00	0.44
2:B:133:LEU:HD23	2:B:133:LEU:C	2.38	0.44
2:B:175:TYR:HB3	4:D:3:PRO:HG3	1.99	0.44
5:N:22:A:H3'	5:N:23:U:H6	1.81	0.44
5:N:26:G:C2'	5:N:27:A:H5'	2.48	0.44
2:B:116:GLU:CD	2:B:116:GLU:H	2.20	0.44
1:A:181:GLN:H	1:A:181:GLN:HE21	1.63	0.44
1:A:283:VAL:O	1:A:284:ARG:HB2	2.18	0.44
2:B:44:LEU:HG	2:B:48:MET:HE1	2.00	0.44
3:C:61:GLU:HB3	4:D:28:LYS:NZ	2.32	0.44
1:A:176:LEU:O	1:A:177:ALA:C	2.56	0.44
2:B:101:LEU:HD11	2:B:133:LEU:HD13	1.99	0.44
2:B:120:ASP:OD2	2:B:122:ARG:HB2	2.17	0.44
1:A:327:MET:HE3	1:A:328:LEU:HD23	1.98	0.43
2:B:226:ASP:HB3	2:B:229:VAL:CG2	2.47	0.43
5:N:23:U:H4'	5:N:26:G:OP1	2.18	0.43
1:A:76:GLU:C	1:A:77:ASN:HD22	2.20	0.43
1:A:195:ARG:HD2	1:A:200:LEU:CD2	2.48	0.43
2:B:154:HIS:O	2:B:158:VAL:HG23	2.17	0.43
1:A:33:VAL:HA	1:A:47:LEU:O	2.18	0.43
1:A:212:LEU:CD2	1:A:305:ASP:HA	2.48	0.43
1:A:212:LEU:HD21	1:A:306:SER:N	2.32	0.43
1:A:217:CYS:O	1:A:221:GLU:HG3	2.18	0.43
1:A:101:LEU:N	1:A:101:LEU:HD12	2.34	0.43
4:D:5:ASP:OD2	4:D:7:ARG:HB2	2.18	0.43
1:A:107:GLU:HB2	1:A:159:ARG:HG2	2.01	0.43
2:B:36:SER:O	2:B:40:GLN:HG3	2.18	0.43
2:B:101:LEU:CD2	2:B:130:VAL:HG13	2.49	0.43
1:A:38:HIS:CE1	1:A:40:LYS:HB2	2.54	0.43
1:A:49:LYS:HB2	1:A:100:TYR:CE1	2.54	0.43
1:A:101:LEU:HB3	1:A:103:PHE:CE1	2.53	0.43
1:A:283:VAL:HB	1:A:289:LEU:HD21	1.99	0.43
2:B:141:LEU:HB3	2:B:146:PHE:CE1	2.54	0.43
1:A:130:MET:HG3	1:A:219:MET:HG3	2.00	0.42
4:D:37:CYS:O	4:D:41:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HB2	1:A:230:GLN:CG	2.50	0.42
1:A:50:VAL:HG11	1:A:59:PHE:CE1	2.55	0.42
2:B:164:VAL:HA	3:C:35:PHE:CB	2.50	0.42
2:B:44:LEU:O	2:B:48:MET:HG3	2.20	0.42
1:A:25:ILE:HG22	1:A:26:GLY:N	2.35	0.42
1:A:127:LYS:HG2	1:A:314:PHE:CZ	2.55	0.42
2:B:184:LEU:HD11	4:D:43:LEU:HD11	2.01	0.42
2:B:209:ASN:O	3:C:41:VAL:N	2.53	0.42
1:A:75:HIS:HB3	1:A:78:VAL:HG23	2.02	0.42
1:A:208:PRO:N	1:A:209:PRO:CD	2.83	0.42
2:B:30:ASP:HB2	2:B:33:LYS:HB2	2.02	0.42
1:A:148:ARG:HB2	1:A:170:LEU:O	2.20	0.41
1:A:52:MET:HE3	1:A:98:SER:HA	2.03	0.41
4:D:27:CYS:SG	4:D:30:CYS:SG	3.18	0.41
1:A:176:LEU:O	1:A:177:ALA:O	2.38	0.41
1:A:288:ALA:O	1:A:292:ILE:HG13	2.20	0.41
2:B:239:HIS:ND1	3:C:51:ARG:NH1	2.68	0.41
4:D:11:TRP:NE1	4:D:12:LYS:HE2	2.34	0.41
1:A:285:ASP:HA	1:A:286:PRO:HD3	1.90	0.41
2:B:12:TRP:CZ3	2:B:68:ARG:HB3	2.54	0.41
2:B:168:LYS:O	2:B:172:GLN:HG3	2.20	0.41
5:N:22:A:H5''	5:N:23:U:C5	2.56	0.41
1:A:110:LEU:O	1:A:114:LEU:HG	2.21	0.41
1:A:123:LEU:HG	1:A:127:LYS:HE3	2.01	0.41
1:A:175:SER:HB2	4:D:11:TRP:HZ2	1.86	0.41
2:B:133:LEU:HD23	2:B:133:LEU:O	2.21	0.41
2:B:208:SER:O	2:B:209:ASN:HB2	2.21	0.41
2:B:20:GLU:O	2:B:25:ARG:HG2	2.21	0.41
5:N:34:G:H4'	5:N:35:A:C5	2.57	0.40
1:A:75:HIS:HB2	1:A:139:TYR:CD2	2.56	0.40
1:A:273:ARG:HG3	1:A:273:ARG:HH11	1.86	0.40
1:A:299:ASP:OD2	1:A:302:GLN:HG3	2.20	0.40
5:N:30:C:N3	5:N:34:G:N2	2.69	0.40
1:A:198:GLU:OE1	1:A:198:GLU:N	2.47	0.40
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.87	0.40
1:A:110:LEU:HB3	1:A:155:VAL:HB	2.04	0.40
1:A:111:ALA:HB2	1:A:152:ALA:C	2.42	0.40
1:A:227:PRO:HB2	1:A:230:GLN:HG2	2.03	0.40
2:B:82:SER:C	2:B:85:PRO:HD2	2.41	0.40
4:D:49:ARG:N	4:D:49:ARG:HE	2.19	0.40
5:N:38:U:O2'	5:N:39:C:H5''	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:21:G:N2	5:N:21:G:N2[4_558]	2.02	0.18
1:A:261:LEU:CD2	1:A:261:LEU:CD2[4_557]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/330 (92%)	268 (88%)	30 (10%)	6 (2%)	7	37
2	B	253/264 (96%)	237 (94%)	15 (6%)	1 (0%)	34	72
3	C	32/36 (89%)	23 (72%)	6 (19%)	3 (9%)	0	10
4	D	48/58 (83%)	43 (90%)	4 (8%)	1 (2%)	7	36
All	All	637/688 (93%)	571 (90%)	55 (9%)	11 (2%)	9	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	177	ALA
1	A	190	VAL
3	C	59	TYR
3	C	60	ASP
1	A	13	CYS
2	B	260	ALA
3	C	64	ASP
4	D	22	CYS
1	A	178	LYS
1	A	286	PRO



### 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	275/291 (94%)	273 (99%)	2 (1%)	84	90
2	B	233/239 (98%)	230 (99%)	3 (1%)	69	82
3	C	31/33 (94%)	28 (90%)	3 (10%)	8	27
4	D	44/52 (85%)	41 (93%)	3 (7%)	16	41
All	All	583/615 (95%)	572 (98%)	11 (2%)	57	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	181	GLN
2	B	10	LYS
2	B	43	ASN
2	B	251	ARG
3	C	44	LYS
3	C	47	LYS
3	C	63	LYS
4	D	24	ASN
4	D	26	TYR
4	D	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	154	ASN
1	A	181	GLN
1	A	187	ASN
1	A	235	GLN
1	A	255	ASN
1	A	258	ASN
1	A	311	ASN

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Mol	Chain	Res	Type
2	B	21	ASN
2	B	39	GLN
2	B	60	ASN
2	B	73	GLN
2	B	97	GLN
2	B	162	GLN
2	B	180	ASN
2	B	190	GLN
2	B	257	ASN
3	C	58	ASN
4	D	17	GLN
4	D	24	ASN
4	D	35	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	N	20/23 (86%)	6 (30%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	N	24	C
5	N	25	U
5	N	27	A
5	N	33	G
5	N	35	A
5	N	38	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	A	186	1	8,10,11	1.38	1 (12%)	10,14,16	3.68	5 (50%)

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
1	TPO	A	186	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	TPO	P-O1P	2.22	1.57	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TPO	O3P-P-O1P	-6.81	84.04	110.68
1	A	186	TPO	O3P-P-OG1	-6.07	78.78	105.99
1	A	186	TPO	O3P-P-O2P	-4.91	88.86	107.64
1	A	186	TPO	OG1-P-O1P	3.39	122.49	109.39
1	A	186	TPO	O2P-P-OG1	2.21	115.89	105.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	186	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	186	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.