



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:12 am BST

PDB ID : 1NVP
Title : HUMAN TFIIA/TBP/DNA COMPLEX
Authors : Bleichenbacher, M.; Tan, S.; Richmond, T.J.
Deposited on : 2003-02-04
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

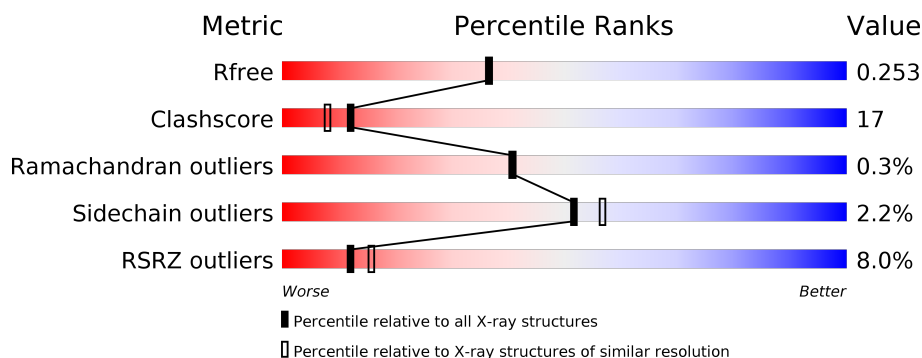
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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 $\leq 5\%$. 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	E	17	<div> <div>6%</div> <div> <div></div> <div>35%</div> <div>47%</div> <div>12%</div> <div>6%</div> </div> </div>
2	F	17	<div> <div>6%</div> <div> <div></div> <div>35%</div> <div>59%</div> <div>6%</div> </div> </div>
3	A	181	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
4	B	57	<div> <div>9%</div> <div> <div></div> <div>54%</div> <div>21%</div> <div>25%</div> </div> </div>
5	C	76	<div> <div>3%</div> <div> <div></div> <div>34%</div> <div>28%</div> <div>38%</div> </div> </div>
6	D	108	<div> <div>16%</div> <div> <div></div> <div>57%</div> <div>31%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3858 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(*GP*GP*GP*GP*GP*GP*GP*CP*TP*AP*TP*AP*AP*AP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	17	Total	C	N	O	P	0	0	0
			359	169	77	97	16			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*CP*CP*CP*CP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	17	Total	C	N	O	P	0	0	0
			332	161	52	103	16			

- Molecule 3 is a protein called TATA box binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	180	Total	C	N	O	S	0	0	0
			1428	927	252	242	7			

- Molecule 4 is a protein called Transcription initiation factor IIA alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	43	Total	C	N	O	S	0	0	0
			352	225	55	70	2			

- Molecule 5 is a protein called Transcription initiation factor IIA beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	47	Total	C	N	O	S	0	0	0
			385	246	67	70	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	301	GLY	-	CLONING ARTIFACT	UNP P52655
C	302	SER	-	CLONING ARTIFACT	UNP P52655

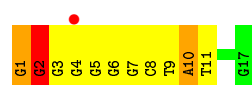
- Molecule 6 is a protein called Transcription initiation factor IIA gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	97	Total	C	N	O	S	0	0	0
			771	491	133	145	2			

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	35	Total	O	0	0
			35	35		
7	F	35	Total	O	0	0
			35	35		
7	A	122	Total	O	0	0
			122	122		
7	B	7	Total	O	0	0
			7	7		
7	C	15	Total	O	0	0
			15	15		
7	D	17	Total	O	0	0
			17	17		

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



C1	C2	T3	T4	T5	T6	A7	T8		C12	C13	C14	C15	C16	C17
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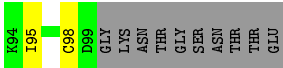
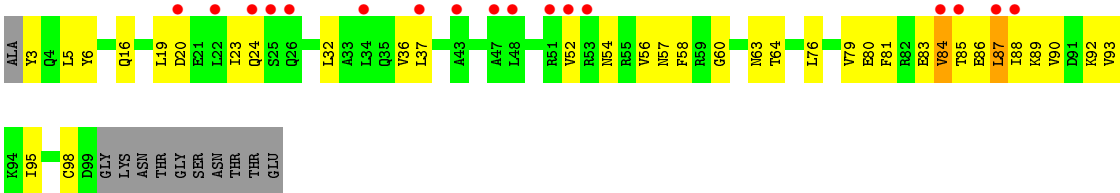
Year	Publications
1959	159
1960	160
1961	161
1962	162
1963	163
1964	164
1965	165
1966	166
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1968	168
1969	169
1970	170
1971	171
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2016	216
2017	217
2018	218
2019	219

ALA	ASN	SER	ALA	ASN	THR	TSN	V10	P11	K12	L13	Y14	R15	S16	V17	I18	E19	D20	V21	T22	R26	E36	K43	E47	M48	M51	GLN	SER	ARG	ALA	VAL	ASP	GLY
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GLY	SER	GLY	ALA	GLU	ASP	GLN	GLN	VAL	GLU	GLU	PRO	LEU	ASN	SER	GLU	ASP	ASP	VAL	SER	ASP	GLU	GLY	GLY	GLN	GLU	LEU	PHE	D30	D31	D32	D33	D34	D35	D36	D37	D38	D39	D40	D41	D42	D43	D44	D45	D46	D47	D48	D49	D50	D51	D52	D53	D54	D55	D56	D57	D58	D59	D60	D61	D62	D63	D64	D65	D66	D67	D68	D69	D70	D71	D72	D73	D74	D75	D76	D77	D78	D79	D80	D81	D82	D83	D84	D85	D86	D87	D88	D89	D90	D91	D92	D93	D94	D95	D96	D97	D98	D99	D100
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● Molecule 6: Transcription initiation factor IIA gamma chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.62Å 90.88Å 125.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.10 39.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.00-2.10) 99.7 (39.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.247 0.234 , 0.253	Depositor DCC
R_{free} test set	3268 reflections (8.09%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3858	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	0.55	0/406	1.06	1/628 (0.2%)
2	F	0.42	0/368	1.05	0/563
3	A	0.43	0/1454	0.67	0/1957
4	B	0.30	0/356	0.53	0/483
5	C	0.38	0/394	0.72	0/528
6	D	0.32	0/781	0.71	2/1061 (0.2%)
All	All	0.41	0/3759	0.78	3/5220 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
2	F	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	87	LEU	N-CA-C	7.14	130.28	111.00
1	E	2	DG	N9-C1'-C2'	5.92	123.85	112.60
6	D	86	GLU	N-CA-C	5.05	124.64	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	DG	Sidechain
1	E	10	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	E	2	DG	Sidechain
2	F	15	DC	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	E	359	0	191	13	0
2	F	332	0	194	15	0
3	A	1428	0	1521	34	0
4	B	352	0	349	7	0
5	C	385	0	367	27	0
6	D	771	0	764	32	0
7	A	122	0	0	0	0
7	B	7	0	0	0	0
7	C	15	0	0	1	0
7	D	17	0	0	0	0
7	E	35	0	0	0	0
7	F	35	0	0	0	0
All	All	3858	0	3386	116	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 17.

All (116) 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)
3:A:302:LEU:HD22	3:A:328:ILE:HD12	1.33	1.06
3:A:204:ILE:HD11	3:A:209:THR:OG1	1.59	1.02
2:F:14:DC:H4'	2:F:15:DC:OP1	1.67	0.93
1:E:4:DG:H4'	1:E:5:DG:OP1	1.70	0.91
6:D:87:LEU:HD11	6:D:89:LYS:HE3	1.54	0.89
5:C:366:ILE:HG21	6:D:52:VAL:HG21	1.59	0.85
3:A:283:TYR:CZ	3:A:285:PRO:HG3	2.16	0.81
3:A:204:ILE:HD12	3:A:237:TYR:OH	1.81	0.79
3:A:204:ILE:O	3:A:204:ILE:HD13	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:267:PRO:HB2	3:A:337:LYS:HB2	1.66	0.76
4:B:43:LYS:O	4:B:47:GLU:HG3	1.84	0.76
1:E:6:DG:H2''	1:E:7:DG:O5'	1.82	0.76
3:A:193:ASN:ND2	3:A:195:LYS:HG2	2.00	0.76
3:A:193:ASN:HD21	3:A:195:LYS:HG2	1.51	0.75
5:C:336:VAL:HG12	6:D:5:LEU:HG	1.68	0.75
5:C:332:GLU:HG2	5:C:334:VAL:HG23	1.74	0.70
5:C:331:THR:OG1	5:C:362:GLY:HA2	1.91	0.70
3:A:302:LEU:HD22	3:A:328:ILE:CD1	2.19	0.67
1:E:3:DG:H2''	1:E:4:DG:C8	2.29	0.67
3:A:278:GLN:NE2	3:A:278:GLN:H	1.93	0.65
2:F:15:DC:H2''	2:F:16:DC:O5'	1.97	0.64
2:F:14:DC:H2''	2:F:15:DC:C6	2.32	0.64
5:C:336:VAL:CG1	6:D:5:LEU:HG	2.28	0.63
2:F:14:DC:H2'	2:F:15:DC:C5	2.33	0.62
2:F:12:DC:H2'	2:F:13:DC:C6	2.34	0.62
1:E:10:DA:H2''	1:E:11:DT:H5'	1.83	0.60
6:D:3:TYR:C	6:D:5:LEU:H	2.04	0.60
5:C:336:VAL:HG11	6:D:5:LEU:O	2.02	0.59
1:E:7:DG:H2''	1:E:8:DC:O5'	2.02	0.59
3:A:159:SER:C	3:A:161:ILE:H	2.06	0.58
5:C:372:GLY:HA2	6:D:58:PHE:O	2.04	0.58
5:C:343:HIS:CD2	7:C:175:HOH:O	2.56	0.57
2:F:14:DC:C2'	2:F:15:DC:C5	2.87	0.57
5:C:332:GLU:HG2	5:C:334:VAL:CG2	2.35	0.57
1:E:6:DG:C2'	1:E:7:DG:O5'	2.52	0.57
2:F:8:DT:H1'	3:A:305:PHE:CZ	2.40	0.56
6:D:32:LEU:O	6:D:36:VAL:HG23	2.05	0.56
5:C:338:GLN:HA	6:D:98:CYS:O	2.06	0.56
1:E:6:DG:H2''	1:E:7:DG:C5'	2.37	0.55
3:A:204:ILE:HD12	3:A:204:ILE:H	1.72	0.55
1:E:8:DC:H2'	1:E:9:DT:C6	2.41	0.55
1:E:2:DG:H2'	1:E:3:DG:C8	2.41	0.55
5:C:366:ILE:HG22	6:D:52:VAL:HG11	1.88	0.54
6:D:87:LEU:HD11	6:D:89:LYS:CE	2.33	0.54
1:E:1:DG:H2'	1:E:2:DG:C8	2.42	0.54
3:A:278:GLN:HG2	3:A:279:GLN:HE21	1.73	0.54
3:A:204:ILE:H	3:A:204:ILE:CD1	2.21	0.54
6:D:83:GLU:O	6:D:85:THR:N	2.40	0.54
3:A:204:ILE:CD1	3:A:209:THR:OG1	2.47	0.54
5:C:374:ALA:HA	6:D:60:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:90:VAL:HG22	6:D:92:LYS:H	1.73	0.53
3:A:304:ILE:N	3:A:304:ILE:HD12	2.23	0.53
6:D:5:LEU:HD13	6:D:98:CYS:SG	2.49	0.52
4:B:18:ILE:O	4:B:22:ILE:HG12	2.10	0.51
6:D:87:LEU:CD1	6:D:89:LYS:HE3	2.35	0.51
3:A:201:ILE:HD12	3:A:201:ILE:N	2.26	0.51
6:D:79:VAL:HG21	6:D:93:VAL:HG12	1.91	0.51
2:F:15:DC:H2''	2:F:16:DC:C5'	2.39	0.51
6:D:5:LEU:HD23	6:D:6:TYR:CZ	2.46	0.51
6:D:54:ASN:ND2	6:D:83:GLU:OE2	2.42	0.50
3:A:204:ILE:N	3:A:204:ILE:CD1	2.74	0.50
3:A:159:SER:HB2	3:A:161:ILE:HG12	1.92	0.50
6:D:83:GLU:O	6:D:84:VAL:C	2.48	0.50
3:A:204:ILE:HD13	3:A:209:THR:H	1.76	0.50
6:D:56:VAL:HG12	6:D:57:ASN:N	2.27	0.50
3:A:188:ARG:HH11	6:D:64:THR:HG21	1.77	0.49
3:A:204:ILE:C	3:A:204:ILE:HD13	2.33	0.49
3:A:228:GLU:HA	3:A:228:GLU:OE1	2.13	0.49
2:F:15:DC:C2'	2:F:16:DC:O5'	2.59	0.49
3:A:278:GLN:H	3:A:278:GLN:HE21	1.59	0.49
2:F:1:DC:H2'	2:F:2:DC:C6	2.48	0.49
3:A:292:ILE:N	3:A:292:ILE:HD12	2.28	0.48
1:E:7:DG:H2''	1:E:8:DC:C5'	2.42	0.48
3:A:159:SER:HB2	3:A:161:ILE:H	1.77	0.48
5:C:359:ASN:HA	5:C:363:ARG:O	2.13	0.48
6:D:20:ASP:HA	6:D:23:ILE:HD12	1.95	0.48
3:A:204:ILE:HD12	3:A:204:ILE:N	2.29	0.48
4:B:43:LYS:HE2	4:B:47:GLU:OE2	2.14	0.48
5:C:333:ASN:HA	5:C:359:ASN:O	2.14	0.48
4:B:17:VAL:O	4:B:21:VAL:HG23	2.14	0.48
2:F:12:DC:H2''	2:F:13:DC:O5'	2.14	0.48
5:C:331:THR:CG2	5:C:359:ASN:OD1	2.62	0.47
6:D:81:PHE:HB2	6:D:88:ILE:HB	1.97	0.47
6:D:79:VAL:HG12	6:D:80:GLU:N	2.30	0.46
2:F:14:DC:C4'	2:F:15:DC:OP1	2.53	0.46
3:A:204:ILE:HD11	3:A:209:THR:HG1	1.75	0.46
5:C:331:THR:HG21	5:C:359:ASN:OD1	2.16	0.46
6:D:80:GLU:HG2	6:D:89:LYS:HG2	1.97	0.45
6:D:16:GLN:HG2	6:D:37:LEU:HD21	1.99	0.45
5:C:369:LYS:HE2	5:C:369:LYS:HB3	1.71	0.45
6:D:63:ASN:OD1	6:D:64:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:DA:H2''	1:E:11:DT:C5'	2.46	0.45
5:C:348:LYS:HZ2	5:C:375:GLU:CD	2.21	0.44
1:E:1:DG:H2''	1:E:2:DG:O5'	2.17	0.44
6:D:79:VAL:HG21	6:D:93:VAL:CG1	2.47	0.44
4:B:26:ARG:NE	4:B:36:GLU:OE2	2.51	0.43
5:C:331:THR:OG1	5:C:362:GLY:CA	2.65	0.43
5:C:331:THR:CG2	5:C:332:GLU:N	2.81	0.43
5:C:366:ILE:HG22	5:C:367:PHE:N	2.33	0.43
3:A:159:SER:C	3:A:161:ILE:N	2.70	0.43
3:A:188:ARG:NH1	6:D:64:THR:HG21	2.33	0.43
4:B:19:GLU:HA	4:B:19:GLU:OE1	2.19	0.43
5:C:335:VAL:HG22	5:C:358:MET:HG2	2.01	0.42
3:A:204:ILE:CD1	3:A:209:THR:H	2.33	0.42
5:C:334:VAL:HG12	5:C:335:VAL:N	2.34	0.42
2:F:7:DA:H2''	2:F:8:DT:H5'	2.00	0.42
3:A:302:LEU:HB2	3:A:304:ILE:HD11	2.00	0.42
6:D:19:LEU:O	6:D:23:ILE:HG13	2.20	0.42
5:C:351:PHE:N	5:C:351:PHE:CD1	2.87	0.41
5:C:331:THR:HG22	5:C:332:GLU:C	2.41	0.41
2:F:14:DC:H2''	2:F:15:DC:C5	2.55	0.41
2:F:4:DT:H2''	2:F:5:DT:H5'	2.03	0.41
3:A:298:PRO:HD3	3:A:323:GLU:HG2	2.02	0.41
4:B:11:PRO:O	4:B:15:ARG:HG2	2.21	0.40
5:C:367:PHE:C	5:C:367:PHE:CD1	2.95	0.40
5:C:335:VAL:HB	6:D:95:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	178/181 (98%)	175 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	41/57 (72%)	40 (98%)	1 (2%)	0	100	100
5	C	45/76 (59%)	43 (96%)	2 (4%)	0	100	100
6	D	95/108 (88%)	87 (92%)	7 (7%)	1 (1%)	14	9
All	All	359/422 (85%)	345 (96%)	13 (4%)	1 (0%)	41	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	84	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	155/156 (99%)	152 (98%)	3 (2%)	57	63
4	B	41/52 (79%)	40 (98%)	1 (2%)	49	53
5	C	40/66 (61%)	39 (98%)	1 (2%)	47	52
6	D	84/97 (87%)	82 (98%)	2 (2%)	49	53
All	All	320/371 (86%)	313 (98%)	7 (2%)	52	57

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	193	ASN
3	A	204	ILE
3	A	278	GLN
4	B	13	LEU
5	C	364	ASP
6	D	24	GLN
6	D	76	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	193	ASN
3	A	278	GLN
3	A	279	GLN
4	B	48	ASN
5	C	352	HIS
6	D	8	ASN
6	D	13	ASN
6	D	31	GLN
6	D	35	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	E	17/17 (100%)	0.45	1 (5%) 22 27	32, 43, 82, 83	0
2	F	17/17 (100%)	0.39	1 (5%) 22 27	34, 46, 87, 88	0
3	A	180/181 (99%)	0.41	6 (3%) 46 53	29, 43, 70, 95	0
4	B	43/57 (75%)	0.64	5 (11%) 4 6	52, 63, 93, 99	0
5	C	47/76 (61%)	0.41	2 (4%) 35 41	43, 67, 82, 100	0
6	D	97/108 (89%)	0.91	17 (17%) 1 1	43, 68, 104, 106	0
All	All	401/456 (87%)	0.56	32 (7%) 12 16	29, 57, 91, 106	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	160	GLY	5.8
6	D	34	LEU	4.7
3	A	159	SER	4.4
6	D	47	ALA	4.1
4	B	15	ARG	3.8
6	D	85	THR	3.7
3	A	338	THR	3.6
4	B	48	ASN	3.5
6	D	52	VAL	3.5
6	D	20	ASP	3.4
6	D	88	ILE	3.4
6	D	26	GLN	3.3
6	D	43	ALA	3.1
6	D	22	LEU	3.0
6	D	87	LEU	2.9
1	E	4	DG	2.8
6	D	24	GLN	2.7
6	D	51	ARG	2.6
4	B	51	MET	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	84	VAL	2.5
2	F	14	DC	2.5
4	B	14	TYR	2.5
6	D	48	LEU	2.5
6	D	53	ARG	2.5
6	D	37	LEU	2.4
6	D	25	SER	2.4
3	A	161	ILE	2.3
5	C	366	ILE	2.2
4	B	11	PRO	2.2
3	A	168	ILE	2.1
5	C	331	THR	2.1
3	A	301	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.