



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:55 PM UTC

PDB ID : 2ASJ / pdb_00002asj
Title : oxoG-modified Preinsertion Binary Complex
Authors : Rechkoblit, O.; Malinina, L.; Cheng, Y.; Kuryavyi, V.; Broyde, S.; Geacintov, N.E.; Patel, D.J.
Deposited on : 2005-08-23
Resolution : 2.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

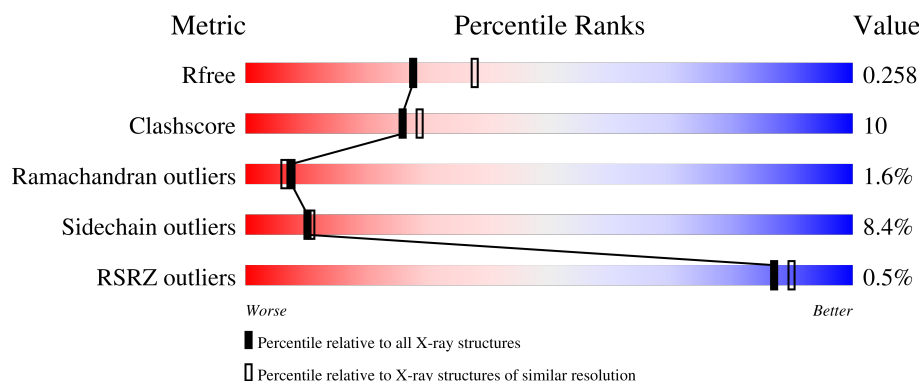
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

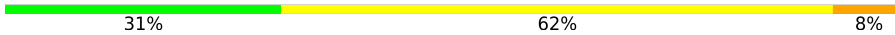
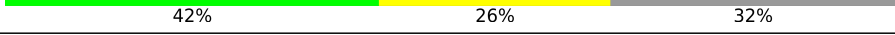
The reported resolution of this entry is 2.35 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	D	13	
1	H	13	
2	E	19	
2	J	19	
3	A	360	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	360	% 69% 22% • 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6677 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*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			
1	H	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			254	123	45	74	12			
2	J	13	Total	C	N	O	P	0	0	0
			254	123	45	74	12			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			
3	B	341	Total	C	N	O	S	0	0	0
			2739	1757	472	504	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP Q97W02
A	-6	SER	-	cloning artifact	UNP Q97W02
A	-5	HIS	-	cloning artifact	UNP Q97W02
A	-4	MET	-	cloning artifact	UNP Q97W02
A	-3	GLY	-	cloning artifact	UNP Q97W02
A	-2	GLY	-	cloning artifact	UNP Q97W02

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q97W02
A	0	GLY	-	cloning artifact	UNP Q97W02
A	1	GLY	-	cloning artifact	UNP Q97W02
B	-7	GLY	-	cloning artifact	UNP Q97W02
B	-6	SER	-	cloning artifact	UNP Q97W02
B	-5	HIS	-	cloning artifact	UNP Q97W02
B	-4	MET	-	cloning artifact	UNP Q97W02
B	-3	GLY	-	cloning artifact	UNP Q97W02
B	-2	GLY	-	cloning artifact	UNP Q97W02
B	-1	GLY	-	cloning artifact	UNP Q97W02
B	0	GLY	-	cloning artifact	UNP Q97W02
B	1001	GLY	-	cloning artifact	UNP Q97W02

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

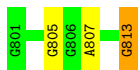
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	11	Total O 11 11	0	0
5	E	9	Total O 9 9	0	0
5	H	10	Total O 10 10	0	0
5	J	8	Total O 8 8	0	0
5	A	45	Total O 45 45	0	0
5	B	61	Total O 61 61	0	0

3 Residue-property plots

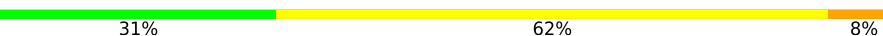
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

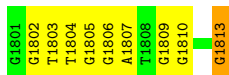
- Molecule 1: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain D: 



- Molecule 1: 5'-D(*GP*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*(DDG))-3'

Chain H: 



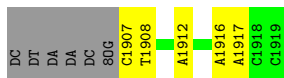
- Molecule 2: 5'-D(*CP*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

Chain E: 



- Molecule 2: 5'-D(*CP*TP*AP*AP*CP*(8OG)*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3'

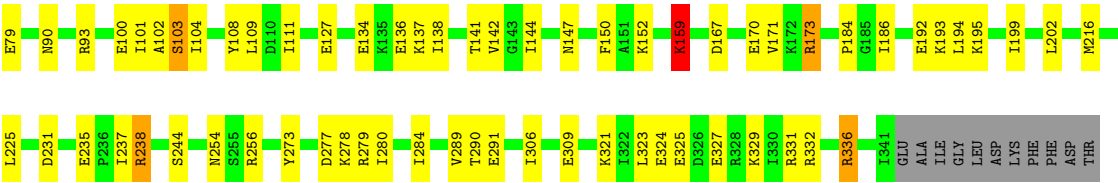
Chain J: 



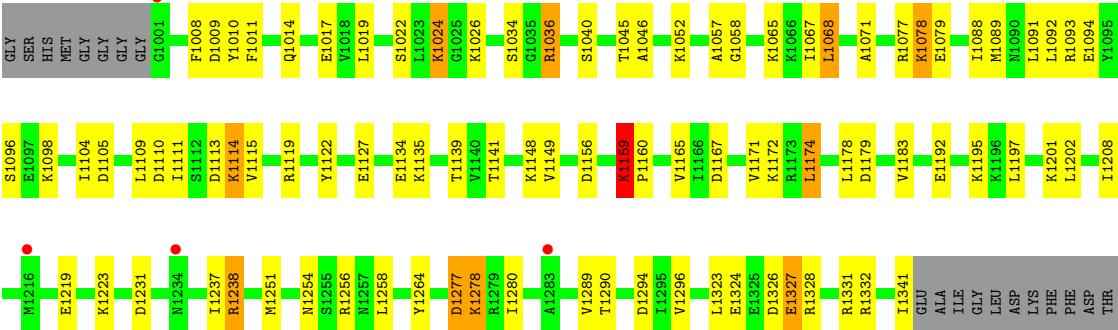
- Molecule 3: DNA polymerase IV

Chain A: 





• Molecule 3: DNA polymerase IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.22Å 182.96Å 52.21Å 90.00° 107.68° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	88.7 (20.00-2.35) 88.6 (20.00-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.246 , 0.318 (Not available) , 0.258	Depositor DCC
R_{free} test set	1878 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.299 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

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

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	D	0.32	0/282	1.05	0/436
1	H	0.37	0/282	1.04	0/436
2	E	0.39	0/283	1.09	0/432
2	J	0.34	0/283	1.02	0/432
3	A	0.69	0/2778	0.93	3/3731 (0.1%)
3	B	0.67	0/2778	0.98	4/3731 (0.1%)
All	All	0.64	0/6686	0.97	7/9198 (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
3	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1011	PHE	N-CA-C	7.07	118.67	110.97
3	A	159	LYS	N-CA-C	6.17	123.44	109.81
3	A	159	LYS	CA-C-N	-5.46	113.02	119.84
3	A	159	LYS	C-N-CA	-5.46	113.02	119.84
3	B	1149	VAL	N-CA-C	5.08	115.31	110.53
3	B	1183	VAL	CA-C-N	5.01	125.24	119.83
3	B	1183	VAL	C-N-CA	5.01	125.24	119.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	69	PRO	Peptide

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	D	272	0	149	4	0
1	H	272	0	149	12	0
2	E	254	0	147	7	0
2	J	254	0	147	7	0
3	A	2739	0	2883	53	0
3	B	2739	0	2880	48	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	45	0	0	3	0
5	B	61	0	0	5	0
5	D	11	0	0	0	0
5	E	9	0	0	1	0
5	H	10	0	0	0	0
5	J	8	0	0	3	0
All	All	6677	0	6355	121	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 10.

All (121) 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:B:1098:LYS:HD3	3:B:1110:ASP:HB3	1.55	0.89
3:A:238:ARG:HH21	3:A:238:ARG:HB2	1.48	0.79
3:B:1014:GLN:HE22	3:B:1139:THR:H	1.30	0.78
1:H:1809:DG:H2''	1:H:1810:DG:H5''	1.67	0.77
3:A:331:ARG:HH21	3:A:332:ARG:HE	1.32	0.76
2:J:1908:DT:OP2	3:B:1332:ARG:HD3	1.86	0.74
3:A:141:THR:OG1	3:A:159:LYS:O	2.06	0.73
1:D:805:DG:H1	2:E:915:DC:H42	1.35	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:256:ARG:HG3	3:A:329:LYS:HA	1.74	0.69
3:A:254:ASN:OD1	3:A:331:ARG:HG3	1.92	0.68
3:B:1096:SER:HB3	3:B:1109:LEU:HG	1.75	0.68
3:A:336:ARG:HH11	3:A:336:ARG:HB2	1.58	0.67
3:A:290:THR:O	5:A:543:HOH:O	2.11	0.66
2:J:1912:DA:N6	5:J:119:HOH:O	2.27	0.65
3:A:273:TYR:OH	3:A:306:ILE:O	2.14	0.65
1:H:1806:DG:H2'	1:H:1807:DA:C8	2.33	0.64
3:A:167:ASP:O	3:A:171:VAL:HG23	1.96	0.64
3:B:1036:ARG:NH2	3:B:1254:ASN:OD1	2.31	0.64
3:B:1078:LYS:HE2	3:B:1104:ILE:HD12	1.79	0.64
3:B:1156:ASP:HA	3:B:1159:LYS:HG3	1.81	0.63
3:A:152:LYS:HD3	3:A:184:PRO:HB3	1.80	0.61
1:H:1803:DT:H72	5:J:39:HOH:O	1.99	0.61
1:D:805:DG:H1	2:E:915:DC:N4	1.99	0.61
3:B:1201:LYS:HB3	5:B:45:HOH:O	2.01	0.60
3:B:1174:LEU:O	3:B:1178:LEU:HB3	2.02	0.59
3:B:1119:ARG:NH2	5:B:69:HOH:O	2.34	0.59
3:B:1017:GLU:HB3	3:B:1024:LYS:HD2	1.85	0.58
3:B:1141:THR:HG21	3:B:1159:LYS:HA	1.85	0.58
3:A:38:GLU:O	3:A:39:ASP:HB2	2.04	0.58
3:B:1135:LYS:HE3	5:B:150:HOH:O	2.04	0.57
1:D:807:DA:H2	2:E:913:DT:H3	1.53	0.57
3:B:1141:THR:OG1	3:B:1159:LYS:O	2.13	0.57
3:B:1289:VAL:HB	3:B:1332:ARG:HB2	1.88	0.56
3:A:100:GLU:HG3	3:A:238:ARG:O	2.06	0.56
2:E:907:DC:N4	3:A:58:GLY:HA2	2.21	0.56
2:E:914:DC:H2'	5:E:505:HOH:O	2.05	0.55
1:H:1813:DDG:H8	1:H:1813:DDG:O5'	2.06	0.55
3:A:336:ARG:HB2	3:A:336:ARG:NH1	2.22	0.55
3:A:69:PRO:O	3:A:71:ALA:N	2.40	0.54
1:H:1802:DG:H2'	1:H:1803:DT:H71	1.89	0.54
3:B:1111:ILE:O	3:B:1115:VAL:HG22	2.08	0.54
3:A:238:ARG:HB2	3:A:238:ARG:NH2	2.20	0.53
3:A:93:ARG:HH21	3:A:101:ILE:HD11	1.71	0.53
3:A:14:GLN:HG2	3:A:138:ILE:HD13	1.89	0.53
3:B:1113:ASP:HB2	3:B:1114:LYS:HE2	1.91	0.53
1:H:1804:DT:H2'	1:H:1805:DG:C8	2.43	0.53
3:A:237:ILE:HG22	3:A:237:ILE:O	2.09	0.52
3:A:102:ALA:O	3:A:103:SER:HB3	2.10	0.52
3:A:291:GLU:OE1	3:A:329:LYS:HB2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:908:DT:H5'	3:A:32:VAL:HG11	1.91	0.51
3:A:17:GLU:HB3	3:A:24:LYS:HE2	1.92	0.51
3:A:279:ARG:O	3:A:280:ILE:HD13	2.11	0.51
2:J:1907:DC:H2'	2:J:1908:DT:H71	1.93	0.50
3:A:76:MET:HG3	3:A:77:ARG:N	2.25	0.50
1:H:1809:DG:H2''	1:H:1810:DG:C5'	2.39	0.50
3:B:1014:GLN:NE2	3:B:1139:THR:H	2.04	0.50
3:B:1294:ASP:HB2	3:B:1328:ARG:HH12	1.76	0.50
3:A:277:ASP:O	3:A:278:LYS:HB2	2.11	0.50
3:B:1068:LEU:HD13	3:B:1071:ALA:HB2	1.93	0.50
3:B:1009:ASP:OD1	3:B:1141:THR:OG1	2.30	0.50
3:A:34:SER:OG	3:A:40:SER:HB2	2.12	0.49
3:B:1088:ILE:O	3:B:1092:LEU:HG	2.13	0.49
2:J:1916:DA:H2''	2:J:1917:DA:O5'	2.13	0.49
3:B:1008:PHE:CZ	3:B:1088:ILE:HG21	2.48	0.49
3:A:186:ILE:HG13	3:A:225:LEU:HD21	1.95	0.48
3:A:291:GLU:HG2	3:A:329:LYS:O	2.13	0.48
3:A:278:LYS:HA	5:A:518:HOH:O	2.12	0.48
3:B:1238:ARG:O	3:B:1238:ARG:HD2	2.13	0.48
3:B:1327:GLU:HG2	5:B:79:HOH:O	2.13	0.48
1:D:813:DDG:H1	2:E:907:DC:H42	1.62	0.48
3:B:1091:LEU:O	3:B:1094:GLU:HG2	2.14	0.48
3:A:36:ARG:NH2	3:A:331:ARG:HG3	2.29	0.47
3:A:108:TYR:OH	3:A:152:LYS:HD2	2.15	0.47
3:B:1251:MET:HA	3:B:1264:TYR:CE1	2.50	0.47
2:J:1907:DC:N4	3:B:1058:GLY:HA2	2.30	0.47
3:A:193:LYS:HG2	3:A:216:MET:HE3	1.97	0.47
3:A:10:TYR:CD2	3:A:48:TYR:HE1	2.32	0.47
3:A:63:GLU:HA	3:A:66:LYS:HE3	1.96	0.47
1:H:1809:DG:C2'	1:H:1810:DG:H5''	2.41	0.46
3:B:1022:SER:O	3:B:1026:LYS:HE2	2.15	0.46
3:B:1219:GLU:O	3:B:1223:LYS:HG3	2.14	0.46
3:A:68:LEU:O	3:A:73:TYR:OH	2.30	0.46
3:B:1148:LYS:HD3	3:B:1237:ILE:HG13	1.98	0.46
1:H:1813:DDG:C6	3:B:1057:ALA:HB1	2.45	0.46
3:B:1172:LYS:HG2	5:B:27:HOH:O	2.16	0.46
3:B:1294:ASP:CB	3:B:1328:ARG:HH12	2.29	0.46
3:A:68:LEU:O	3:A:69:PRO:O	2.35	0.45
3:A:170:GLU:HG3	3:A:173:ARG:NH1	2.31	0.45
3:B:1008:PHE:CD2	3:B:1105:ASP:HA	2.51	0.45
3:A:147:ASN:OD1	3:A:150:PHE:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:238:ARG:H	3:A:238:ARG:HG3	1.64	0.45
3:B:1256:ARG:NH1	3:B:1328:ARG:O	2.50	0.45
3:A:90:ASN:HA	3:A:93:ARG:HD2	1.98	0.44
3:B:1277:ASP:O	3:B:1278:LYS:HB2	2.17	0.44
3:A:32:VAL:O	3:A:41:GLY:HA3	2.17	0.44
3:A:6:VAL:HG22	3:A:142:VAL:HG22	2.00	0.44
3:A:9:ASP:O	3:A:10:TYR:C	2.62	0.42
3:B:1167:ASP:O	3:B:1171:VAL:HG23	2.19	0.42
3:A:192:GLU:HA	3:A:195:LYS:HB3	2.01	0.42
3:A:321:LYS:HG2	3:A:325:GLU:OE2	2.19	0.42
3:A:46:ALA:HB1	3:A:50:ALA:HB3	2.00	0.42
3:B:1296:VAL:HG21	3:B:1326:ASP:OD2	2.19	0.42
3:A:194:LEU:HB3	3:A:199:ILE:HB	2.02	0.42
3:B:1019:LEU:HD23	3:B:1077:ARG:HH22	1.85	0.42
3:B:1034:SER:C	3:B:1036:ARG:H	2.28	0.42
1:H:1804:DT:H2''	1:H:1805:DG:H5'	2.01	0.42
3:B:1045:THR:HG22	3:B:1046:ALA:N	2.35	0.42
3:B:1159:LYS:CB	3:B:1160:PRO:HD3	2.49	0.41
3:B:1159:LYS:HB3	3:B:1160:PRO:HD3	2.02	0.41
3:A:2:ILE:HG22	3:A:111:ILE:HG13	2.02	0.41
3:A:244:SER:HB2	3:A:336:ARG:HE	1.85	0.41
3:B:1089:MET:O	3:B:1093:ARG:HG3	2.21	0.41
1:H:1804:DT:H2'	1:H:1805:DG:H8	1.84	0.41
3:A:50:ALA:O	3:A:55:VAL:HB	2.21	0.41
1:H:1809:DG:C2	2:J:1912:DA:C2	3.09	0.40
3:A:136:GLU:O	3:A:137:LYS:HB2	2.20	0.40
3:B:1009:ASP:C	3:B:1010:TYR:CD2	3.00	0.40
3:B:1122:TYR:HD1	3:B:1165:VAL:HG23	1.86	0.40
2:J:1908:DT:O4	5:J:43:HOH:O	2.16	0.40
3:A:289:VAL:HG12	5:A:543:HOH:O	2.21	0.40
3:B:1251:MET:HG3	3:B:1331:ARG:O	2.21	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	339/360 (94%)	311 (92%)	21 (6%)	7 (2%)	5	4
3	B	339/360 (94%)	321 (95%)	14 (4%)	4 (1%)	10	9
All	All	678/720 (94%)	632 (93%)	35 (5%)	11 (2%)	7	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	36	ARG
3	A	69	PRO
3	A	159	LYS
3	B	1159	LYS
3	B	1277	ASP
3	A	231	ASP
3	A	103	SER
3	B	1052	LYS
3	A	70	ASN
3	B	1278	LYS
3	A	104	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	299/311 (96%)	277 (93%)	22 (7%)	13	14
3	B	299/311 (96%)	271 (91%)	28 (9%)	8	8
All	All	598/622 (96%)	548 (92%)	50 (8%)	10	11

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	ILE
3	A	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	23	LEU
3	A	67	ILE
3	A	70	ASN
3	A	76	MET
3	A	79	GLU
3	A	109	LEU
3	A	127	GLU
3	A	134	GLU
3	A	144	ILE
3	A	159	LYS
3	A	173	ARG
3	A	202	LEU
3	A	235	GLU
3	A	238	ARG
3	A	284	ILE
3	A	309	GLU
3	A	323	LEU
3	A	324	GLU
3	A	327	GLU
3	A	336	ARG
3	B	1024	LYS
3	B	1036	ARG
3	B	1040	SER
3	B	1065	LYS
3	B	1067	ILE
3	B	1068	LEU
3	B	1078	LYS
3	B	1079	GLU
3	B	1114	LYS
3	B	1127	GLU
3	B	1134	GLU
3	B	1159	LYS
3	B	1174	LEU
3	B	1179	ASP
3	B	1192	GLU
3	B	1195	LYS
3	B	1197	LEU
3	B	1202	LEU
3	B	1208	ILE
3	B	1231	ASP
3	B	1238	ARG
3	B	1258	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1280	ILE
3	B	1290	THR
3	B	1323	LEU
3	B	1324	GLU
3	B	1327	GLU
3	B	1341	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	70	ASN
3	A	304	HIS
3	B	1014	GLN
3	B	1070	ASN
3	B	1082	GLN
3	B	1304	HIS
3	B	1320	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are 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	DDG	D	813	1,4,2	20,23,24	0.45	0	27,33,36	0.82	1 (3%)
1	DDG	H	1813	1,4,2	20,23,24	0.62	0	27,33,36	1.17	2 (7%)

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	DDG	D	813	1,4,2	-	0/7/18/19	0/3/3/3
1	DDG	H	1813	1,4,2	-	0/7/18/19	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1813	DDG	C3'-C2'-C1'	2.25	105.47	102.87
1	D	813	DDG	O4'-C1'-C2'	2.18	109.00	106.41
1	H	1813	DDG	C4'-O4'-C1'	2.10	111.79	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	813	DDG	1	0
1	H	1813	DDG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [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(Å²)	Q<0.9	
1	D	12/13 (92%)	0.27	0	100	100	35, 57, 60, 60	0
1	H	12/13 (92%)	0.06	0	100	100	34, 43, 51, 53	0
2	E	13/19 (68%)	0.39	0	100	100	37, 53, 63, 63	0
2	J	13/19 (68%)	0.15	0	100	100	32, 38, 56, 58	0
3	A	341/360 (94%)	0.35	0	100	100	45, 55, 65, 70	0
3	B	341/360 (94%)	0.28	4 (1%)	76	81	45, 55, 64, 69	0
All	All	732/784 (93%)	0.31	4 (0%)	87	90	32, 55, 65, 70	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1234	ASN	2.9
3	B	1216	MET	2.6
3	B	1283	ALA	2.3
3	B	1001	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	DDG	D	813	21/22	0.87	0.10	32,39,40,40	0
1	DDG	H	1813	21/22	0.87	0.10	38,38,41,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	CA	B	1415	1/1	0.81	0.22	52,52,52,52	0
4	CA	E	416	1/1	0.95	0.08	75,75,75,75	0
4	CA	A	415	1/1	0.98	0.19	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.