



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:53 PM GMT

PDB ID : 4G3I  
Title : Crystal structure of Dpo4 in complex with DNA duplex  
Authors : Yan, Y.Y.; Gan, J.H.; Huang, Z.  
Deposited on : 2012-07-14  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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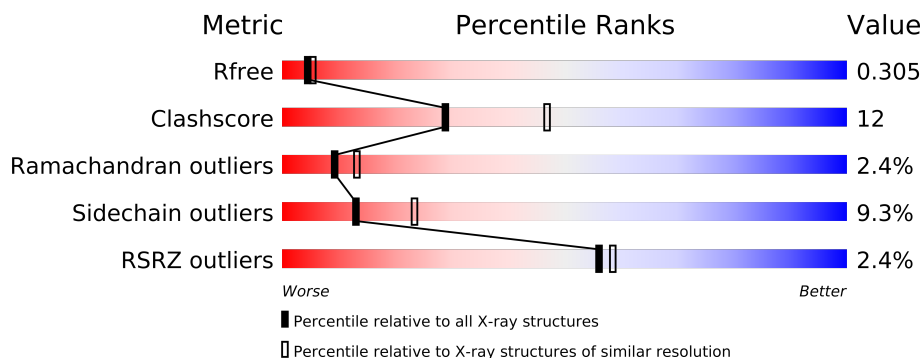
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	16	
1	E	16	
2	D	13	
2	F	13	
3	A	342	
3	B	342	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CA	B	401	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6238 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			
1	E	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
2	F	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	342	Total	C	N	O	S	0	0	0
			2750	1763	473	507	7			
3	B	341	Total	C	N	O	S	0	0	0
			2744	1760	472	505	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q97W02
B	0	SER	-	EXPRESSION TAG	UNP Q97W02

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

- Molecule 5 is water.

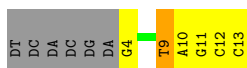
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	O 1	0	0
5	A	16	Total 16	O 16	0	0
5	B	3	Total 3	O 3	0	0

### 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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA

Chain C: 



- Molecule 1: DNA

Chain E: 



- Molecule 2: DNA

Chain D: 



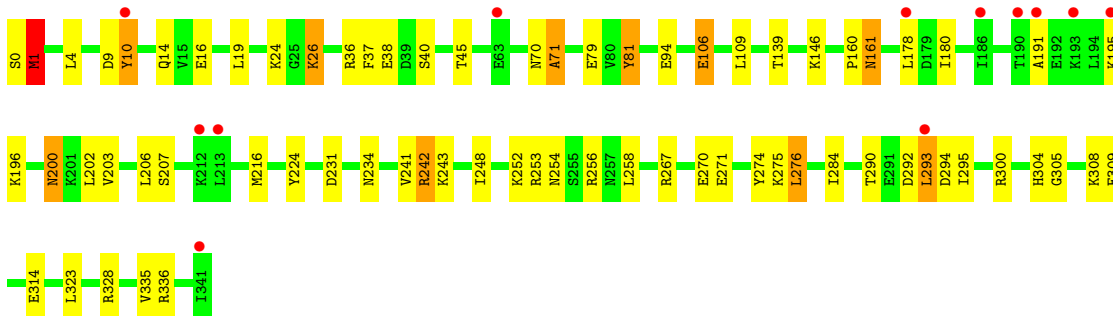
- Molecule 2: DNA

Chain F: 



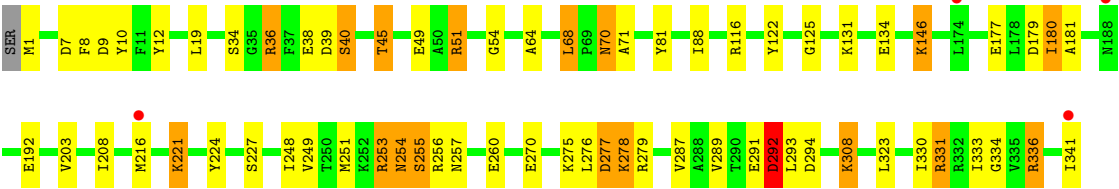
- Molecule 3: DNA polymerase IV

Chain A: 



- Molecule 3: DNA polymerase IV

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.47Å 52.63Å 99.44Å 75.40° 80.35° 70.97°	Depositor
Resolution (Å)	95.81 – 2.50 28.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (95.81-2.50) 97.2 (28.39-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.78 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.241 , 0.294 0.259 , 0.305	Depositor DCC
$R_{free}$ test set	1650 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 11.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 32534 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6238	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: 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	C	1.38	1/220 (0.5%)	2.10	7/337 (2.1%)
1	E	1.30	0/220	2.32	16/337 (4.7%)
2	D	1.35	0/183	2.15	10/281 (3.6%)
2	F	1.32	1/183 (0.5%)	2.28	16/281 (5.7%)
3	A	0.84	2/2789 (0.1%)	0.85	1/3744 (0.0%)
3	B	0.86	0/2783	0.86	1/3736 (0.0%)
All	All	0.93	4/6378 (0.1%)	1.15	51/8716 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	8	DT	C5-C7	5.34	1.53	1.50
3	A	106	GLU	CB-CG	5.24	1.62	1.52
3	A	79	GLU	CG-CD	5.09	1.59	1.51
1	C	11	DG	C3'-O3'	-5.01	1.37	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	DC	O4'-C4'-C3'	-10.35	99.79	106.00
2	D	7	DC	N3-C2-O2	-10.15	114.79	121.90
1	E	7	DC	O4'-C1'-N1	9.74	114.82	108.00
2	D	7	DC	N1-C2-O2	9.47	124.58	118.90
1	C	12	DC	N1-C2-O2	9.30	124.48	118.90
1	E	8	DT	O4'-C1'-N1	9.15	114.40	108.00
1	C	9	DT	O4'-C1'-N1	8.90	114.23	108.00
1	E	8	DT	C3'-C2'-C1'	-8.28	92.56	102.50
2	F	10	DC	C1'-O4'-C4'	-8.23	101.87	110.10
1	E	6	DC	P-O3'-C3'	8.02	129.33	119.70
1	E	6	DC	N1-C2-O2	8.00	123.70	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	DG	C3'-C2'-C1'	-7.98	92.92	102.50
1	E	8	DT	C1'-O4'-C4'	-7.92	102.18	110.10
2	F	6	DG	C5-C6-N1	7.79	115.40	111.50
1	E	12	DC	N3-C4-C5	7.55	124.92	121.90
1	C	13	DC	O4'-C1'-N1	-7.51	102.74	108.00
2	D	11	DA	P-O3'-C3'	7.10	128.22	119.70
2	F	6	DG	N1-C6-O6	-6.74	115.86	119.90
1	E	13	DC	O4'-C1'-C2'	6.67	111.24	105.90
1	E	6	DC	N3-C2-O2	-6.48	117.36	121.90
2	F	8	DT	N3-C4-O4	6.47	123.78	119.90
1	C	12	DC	N3-C2-O2	-6.29	117.50	121.90
1	E	5	DT	C4-C5-C7	6.25	122.75	119.00
2	F	8	DT	C5-C4-O4	-6.21	120.56	124.90
2	F	7	DC	O5'-P-OP2	-6.16	100.16	105.70
2	D	6	DG	C1'-O4'-C4'	-6.13	103.97	110.10
2	F	12	DG	C8-N9-C4	-6.06	103.98	106.40
2	D	8	DT	P-O3'-C3'	6.00	126.90	119.70
2	F	8	DT	C1'-O4'-C4'	-5.67	104.43	110.10
2	D	10	DC	P-O3'-C3'	5.67	126.50	119.70
3	B	7	ASP	CB-CG-OD1	5.63	123.37	118.30
2	F	7	DC	P-O3'-C3'	5.62	126.44	119.70
2	F	6	DG	C6-C5-N7	5.54	133.73	130.40
1	E	10	DA	N1-C6-N6	5.53	121.92	118.60
2	D	5	DG	N9-C1'-C2'	5.50	123.06	112.60
1	E	10	DA	P-O5'-C5'	-5.44	112.19	120.90
1	E	9	DT	O4'-C1'-N1	-5.42	104.20	108.00
2	D	7	DC	C2-N1-C1'	5.42	124.76	118.80
2	D	9	DA	P-O3'-C3'	5.41	126.19	119.70
2	F	10	DC	O4'-C1'-N1	5.38	111.77	108.00
1	E	10	DA	N9-C4-C5	-5.36	103.66	105.80
1	E	10	DA	C5-C6-N6	-5.32	119.45	123.70
2	F	12	DG	C5-C6-O6	-5.30	125.42	128.60
2	D	6	DG	P-O3'-C3'	5.22	125.97	119.70
2	F	5	DG	O4'-C4'-C3'	-5.22	102.41	104.50
1	C	12	DC	C2-N1-C1'	5.21	124.53	118.80
3	A	202	LEU	CA-CB-CG	5.19	127.23	115.30
2	F	7	DC	C2-N3-C4	-5.16	117.32	119.90
2	F	6	DG	C6-N1-C2	-5.12	122.03	125.10
2	F	6	DG	C1'-O4'-C4'	-5.01	105.09	110.10
1	E	5	DT	C6-C5-C7	-5.01	119.90	122.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	198	0	0	1	0
1	E	198	0	0	0	0
2	D	163	0	0	4	0
2	F	163	0	0	2	0
3	A	2750	0	0	34	0
3	B	2744	0	0	38	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
All	All	6238	0	0	74	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:254:ASN:CB	3:B:330:ILE:O	2.22	0.87
3:A:294:ASP:CB	3:A:328:ARG:NH1	2.50	0.74
3:B:256:ARG:O	3:B:323:LEU:CD2	2.36	0.74
2:D:8:DT:O3'	3:A:242:ARG:NH1	2.21	0.72
3:B:254:ASN:N	3:B:254:ASN:OD1	2.22	0.71
2:D:8:DT:OP2	3:A:336:ARG:NH2	2.25	0.70
3:B:116:ARG:NH1	3:B:116:ARG:CB	2.60	0.65
2:F:8:DT:OP2	3:B:336:ARG:NH2	2.33	0.62
2:D:9:DA:OP1	3:A:242:ARG:NH1	2.33	0.61
3:A:200:ASN:ND2	3:A:200:ASN:N	2.47	0.60
3:A:309:GLU:OE1	3:A:309:GLU:N	2.35	0.59
3:A:275:LYS:O	3:A:276:LEU:C	2.43	0.57
2:F:10:DC:C2'	2:F:11:DA:C8	2.89	0.56
3:B:255:SER:CB	3:B:260:GLU:OE1	2.54	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:180:ILE:CG2	3:B:181:ALA:N	2.68	0.55
3:B:116:ARG:CB	3:B:116:ARG:CZ	2.85	0.55
3:A:242:ARG:NH1	3:A:242:ARG:CG	2.71	0.54
3:A:294:ASP:OD2	3:A:328:ARG:NH2	2.41	0.54
2:D:9:DA:P	3:A:242:ARG:NH1	2.81	0.54
3:B:12:TYR:CB	3:B:45:THR:CG2	2.86	0.54
3:A:14:GLN:NE2	3:A:139:THR:N	2.55	0.53
3:A:9:ASP:O	3:A:10:TYR:C	2.47	0.53
3:B:38:GLU:O	3:B:39:ASP:CB	2.56	0.52
3:A:160:PRO:O	3:A:161:ASN:O	2.28	0.52
3:B:9:ASP:O	3:B:10:TYR:C	2.48	0.51
3:A:290:THR:OG1	3:A:292:ASP:OD2	2.29	0.50
3:A:146:LYS:NZ	3:A:231:ASP:OD2	2.44	0.50
3:A:203:VAL:O	3:A:206:LEU:N	2.45	0.50
3:A:16:GLU:OE2	3:A:81:TYR:OH	2.29	0.50
3:A:0:SER:O	3:A:1:MET:CB	2.59	0.50
3:A:10:TYR:O	3:A:10:TYR:CD1	2.65	0.49
3:A:304:HIS:CD2	3:A:305:GLY:O	2.65	0.49
3:B:34:SER:OG	3:B:40:SER:OG	2.31	0.49
3:B:254:ASN:CA	3:B:330:ILE:O	2.61	0.49
3:B:251:MET:CE	3:B:330:ILE:CG2	2.91	0.48
1:C:9:DT:C2'	1:C:10:DA:OP2	2.61	0.48
3:A:300:ARG:NH1	3:A:314:GLU:OE1	2.48	0.47
3:A:4:LEU:O	3:A:109:LEU:N	2.46	0.46
3:B:122:TYR:O	3:B:125:GLY:N	2.49	0.46
3:B:254:ASN:ND2	3:B:331:ARG:CD	2.79	0.45
3:A:304:HIS:CD2	3:A:304:HIS:C	2.90	0.45
3:B:1:MET:CE	3:B:146:LYS:O	2.65	0.45
3:B:8:PHE:CZ	3:B:88:ILE:CG2	3.00	0.45
3:B:253:ARG:O	3:B:254:ASN:C	2.55	0.45
3:A:37:PHE:CE1	3:A:40:SER:CB	2.99	0.44
3:B:289:VAL:O	3:B:331:ARG:N	2.51	0.44
3:B:51:ARG:O	3:B:54:GLY:N	2.50	0.44
3:B:292:ASP:OD1	3:B:292:ASP:N	2.51	0.44
3:A:191:ALA:O	3:A:195:LYS:N	2.50	0.44
3:B:277:ASP:O	3:B:278:LYS:CB	2.66	0.44
3:B:270:GLU:OE1	3:B:308:LYS:NZ	2.50	0.44
3:A:10:TYR:O	3:A:10:TYR:CG	2.69	0.44
3:A:160:PRO:O	3:A:161:ASN:C	2.55	0.43
3:B:278:LYS:CE	3:B:278:LYS:CA	2.96	0.43
3:B:275:LYS:O	3:B:279:ARG:NH2	2.51	0.43
3:B:179:ASP:O	3:B:180:ILE:C	2.57	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:36:ARG:NH1	3:B:331:ARG:CD	2.82	0.43
3:B:12:TYR:CD1	3:B:12:TYR:N	2.88	0.42
3:B:64:ALA:O	3:B:68:LEU:N	2.52	0.42
3:A:292:ASP:OD1	3:A:328:ARG:NH1	2.53	0.42
3:A:292:ASP:O	3:A:293:LEU:CB	2.68	0.42
3:B:81:TYR:N	3:B:81:TYR:CD1	2.86	0.42
3:A:256:ARG:NH2	3:A:323:LEU:O	2.52	0.41
3:A:270:GLU:OE2	3:A:308:LYS:NZ	2.53	0.41
3:B:70:ASN:ND2	3:B:70:ASN:O	2.53	0.41
3:A:234:ASN:CG	3:A:234:ASN:O	2.58	0.41
3:B:49:GLU:N	3:B:49:GLU:OE1	2.54	0.41
3:B:287:VAL:O	3:B:334:GLY:N	2.54	0.41
3:A:81:TYR:CD1	3:A:81:TYR:N	2.85	0.41
3:B:291:GLU:O	3:B:293:LEU:N	2.55	0.40
3:B:276:LEU:O	3:B:277:ASP:C	2.60	0.40
3:A:70:ASN:C	3:A:71:ALA:O	2.60	0.40
3:B:333:ILE:O	3:B:333:ILE:CG2	2.69	0.40
3:B:221:LYS:O	3:B:224:TYR:N	2.55	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	340/342 (99%)	302 (89%)	26 (8%)	12 (4%)	6	7
3	B	339/342 (99%)	304 (90%)	31 (9%)	4 (1%)	19	32
All	All	679/684 (99%)	606 (89%)	57 (8%)	16 (2%)	9	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	161	ASN
3	A	295	ILE

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Mol	Chain	Res	Type
3	A	26	LYS
3	A	216	MET
3	B	71	ALA
3	B	277	ASP
3	A	36	ARG
3	A	1	MET
3	A	10	TYR
3	A	293	LEU
3	B	292	ASP
3	A	71	ALA
3	A	252	LYS
3	A	274	TYR
3	A	276	LEU
3	B	180	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	301/301 (100%)	275 (91%)	26 (9%)	15	27
3	B	300/301 (100%)	270 (90%)	30 (10%)	11	20
All	All	601/602 (100%)	545 (91%)	56 (9%)	13	23

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	19	LEU
3	A	24	LYS
3	A	26	LYS
3	A	38	GLU
3	A	45	THR
3	A	81	TYR
3	A	94	GLU
3	A	106	GLU
3	A	178	LEU
3	A	180	ILE

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Mol	Chain	Res	Type
3	A	196	LYS
3	A	200	ASN
3	A	207	SER
3	A	224	TYR
3	A	241	VAL
3	A	242	ARG
3	A	243	LYS
3	A	248	ILE
3	A	253	ARG
3	A	254	ASN
3	A	258	LEU
3	A	267	ARG
3	A	271	GLU
3	A	284	ILE
3	A	335	VAL
3	B	19	LEU
3	B	36	ARG
3	B	40	SER
3	B	45	THR
3	B	51	ARG
3	B	68	LEU
3	B	70	ASN
3	B	131	LYS
3	B	134	GLU
3	B	146	LYS
3	B	177	GLU
3	B	192	GLU
3	B	203	VAL
3	B	208	ILE
3	B	216	MET
3	B	221	LYS
3	B	227	SER
3	B	248	ILE
3	B	249	VAL
3	B	253	ARG
3	B	254	ASN
3	B	255	SER
3	B	257	ASN
3	B	278	LYS
3	B	292	ASP
3	B	294	ASP
3	B	308	LYS

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Mol	Chain	Res	Type
3	B	331	ARG
3	B	336	ARG
3	B	341	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	10/16 (62%)	-0.09	0 100 100	22, 46, 61, 62	0
1	E	10/16 (62%)	0.05	0 100 100	21, 46, 61, 62	0
2	D	8/13 (61%)	0.27	0 100 100	26, 29, 50, 51	0
2	F	8/13 (61%)	0.22	0 100 100	25, 28, 50, 51	0
3	A	342/342 (100%)	0.49	12 (3%) 42 43	10, 30, 52, 72	1 (0%)
3	B	341/342 (99%)	0.39	4 (1%) 75 77	11, 30, 51, 62	0
All	All	719/742 (96%)	0.42	16 (2%) 56 61	10, 30, 54, 72	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	341	ILE	3.9
3	A	341	ILE	3.4
3	A	293	LEU	3.3
3	B	216	MET	3.3
3	A	193	LYS	2.9
3	B	188	ASN	2.7
3	A	10	TYR	2.6
3	A	178	LEU	2.5
3	A	63	GLU	2.4
3	A	191	ALA	2.3
3	B	174	LEU	2.3
3	A	212	LYS	2.2
3	A	195	LYS	2.2
3	A	190	THR	2.2
3	A	186	ILE	2.1
3	A	213	LEU	2.1



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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	B	401	1/1	0.27	7.04	99,99,99,99	0
4	CA	A	401	1/1	0.16	0.32	126,126,126,126	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.