



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:12 PM BST

PDB ID : 5NKK  
Title : SMG8-SMG9 complex GDP bound  
Authors : Li, L.; Basquin, J.; Conti, E.  
Deposited on : 2017-03-31  
Resolution : 2.64 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.

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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 : 2.13.1  
buster-report : 1.1.7 (2018)  
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) : 2.13.1

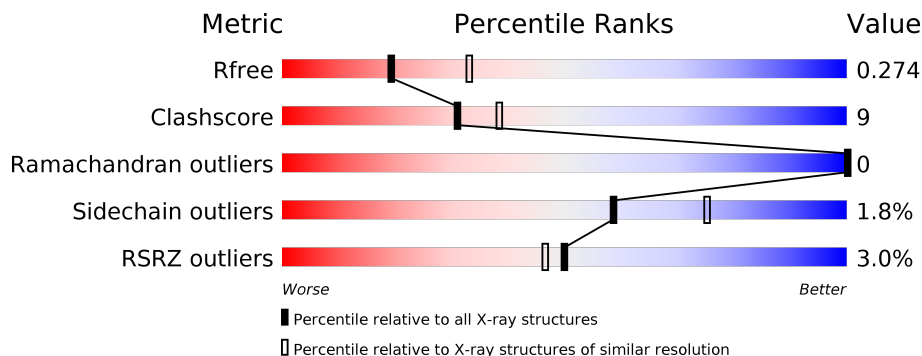
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 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	A	429	<p>2% 66% 13% 21%</p>
1	C	429	<p>3% 65% 12% 23%</p>
1	E	429	<p>2% 66% 14% 19%</p>
2	B	317	<p>2% 57% 24% 19%</p>
2	D	317	<p>2% 58% 23% 19%</p>
2	F	317	<p>4% 64% 15% 20%</p>

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 13739 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 Protein smg-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2597	1631	452	494	20	0	0	0
1	C	330	2517	1580	435	484	18	0	0	0
1	E	347	2608	1638	444	507	19	0	0	0

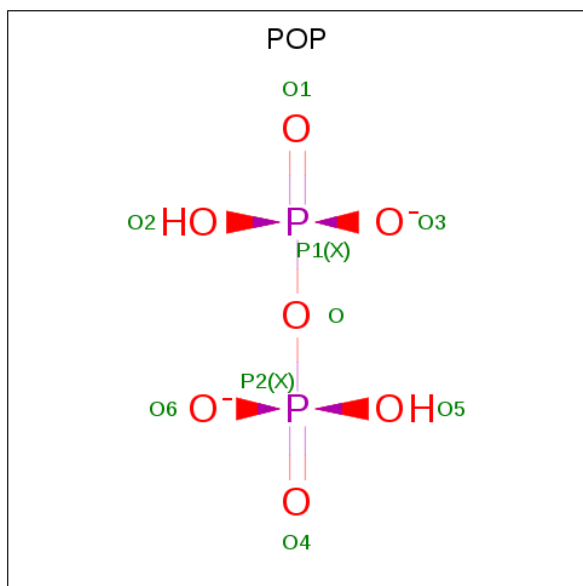
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP O62301
A	425	HIS	-	expression tag	UNP O62301
A	426	HIS	-	expression tag	UNP O62301
A	427	HIS	-	expression tag	UNP O62301
A	428	HIS	-	expression tag	UNP O62301
A	429	HIS	-	expression tag	UNP O62301
C	424	HIS	-	expression tag	UNP O62301
C	425	HIS	-	expression tag	UNP O62301
C	426	HIS	-	expression tag	UNP O62301
C	427	HIS	-	expression tag	UNP O62301
C	428	HIS	-	expression tag	UNP O62301
C	429	HIS	-	expression tag	UNP O62301
E	424	HIS	-	expression tag	UNP O62301
E	425	HIS	-	expression tag	UNP O62301
E	426	HIS	-	expression tag	UNP O62301
E	427	HIS	-	expression tag	UNP O62301
E	428	HIS	-	expression tag	UNP O62301
E	429	HIS	-	expression tag	UNP O62301

- Molecule 2 is a protein called Protein smg-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S	0	0	0
			1960	1253	331	367	9			
2	D	258	Total	C	N	O	S	0	0	0
			1975	1259	330	377	9			
2	F	253	Total	C	N	O	S	0	0	0
			1872	1191	312	361	8			

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



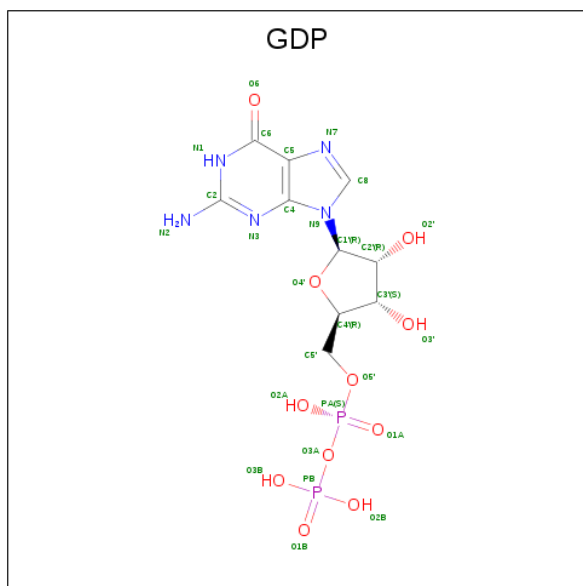
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	O P	0	0
			9	7 2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	F	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

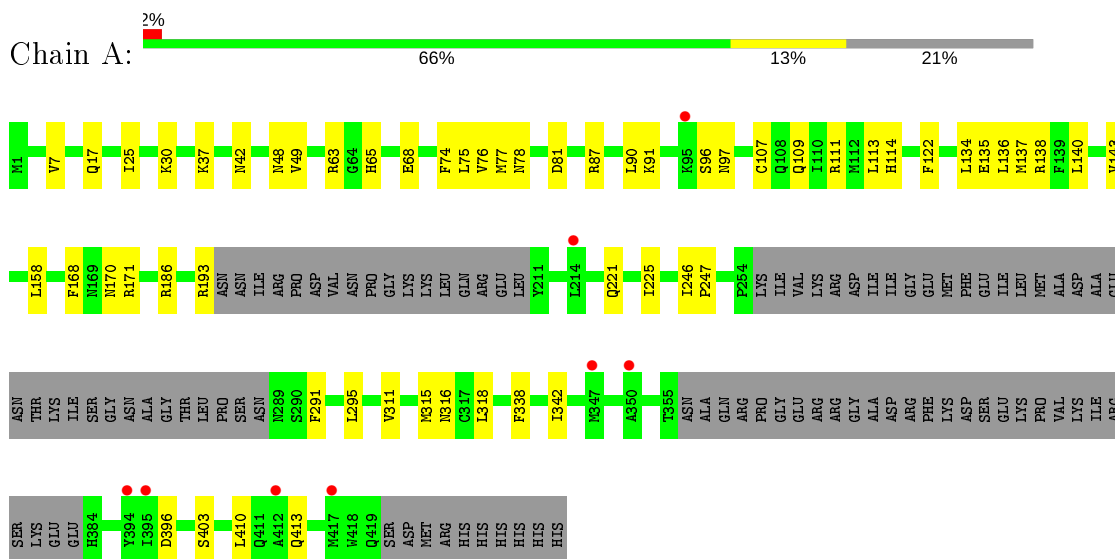
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	33	Total O 33 33	0	0
7	C	36	Total O 36 36	0	0
7	D	20	Total O 20 20	0	0
7	E	20	Total O 20 20	0	0
7	F	12	Total O 12 12	0	0

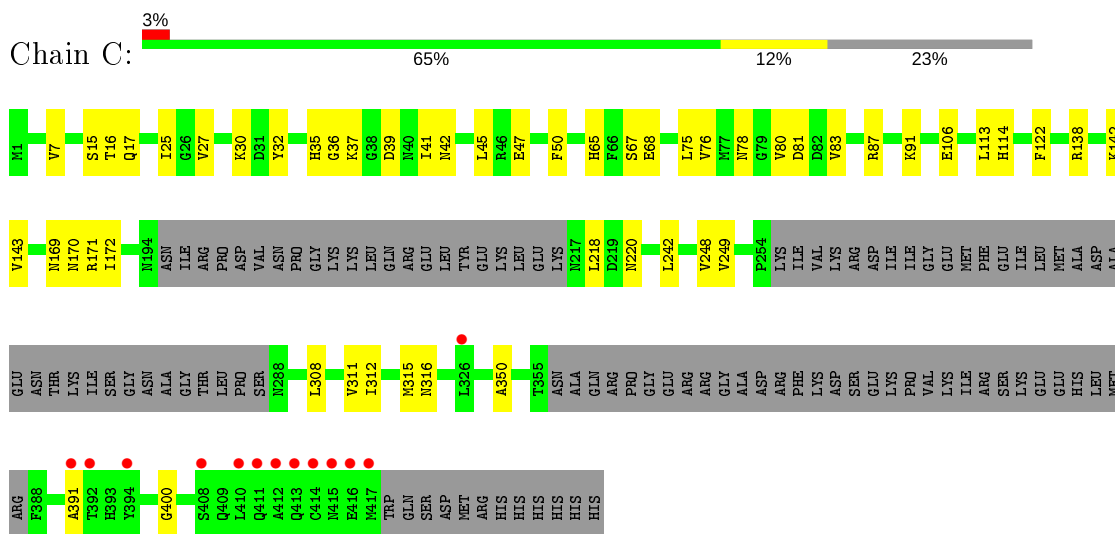
### 3 Residue-property plots [i](#)

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: Protein smg-8

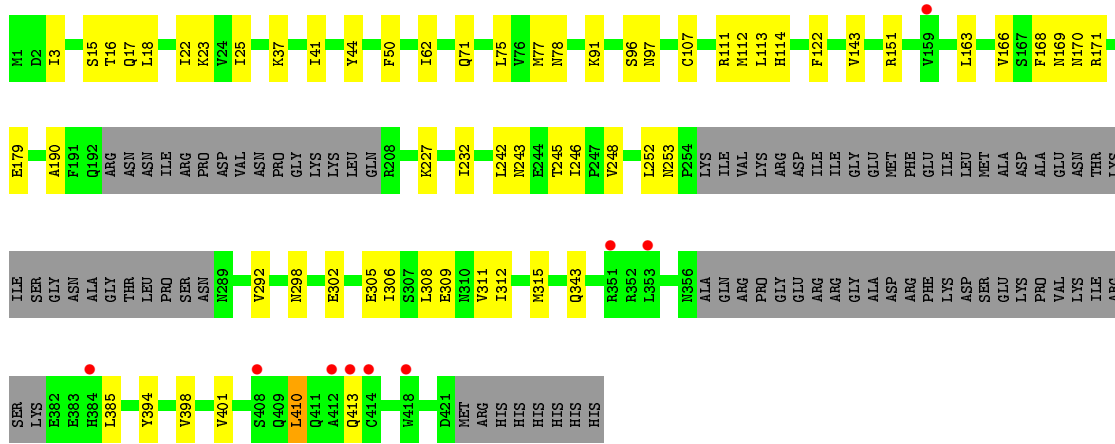


- Molecule 1: Protein smg-8

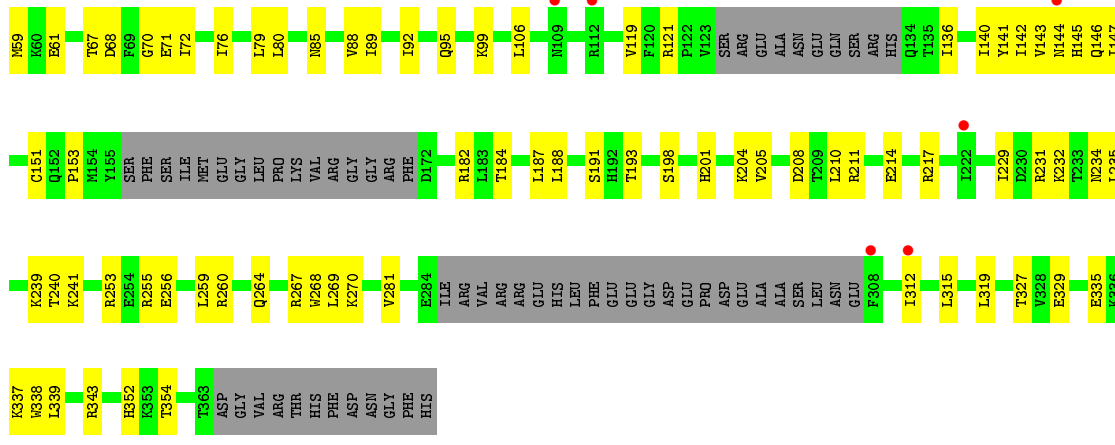


- Molecule 1: Protein smg-8

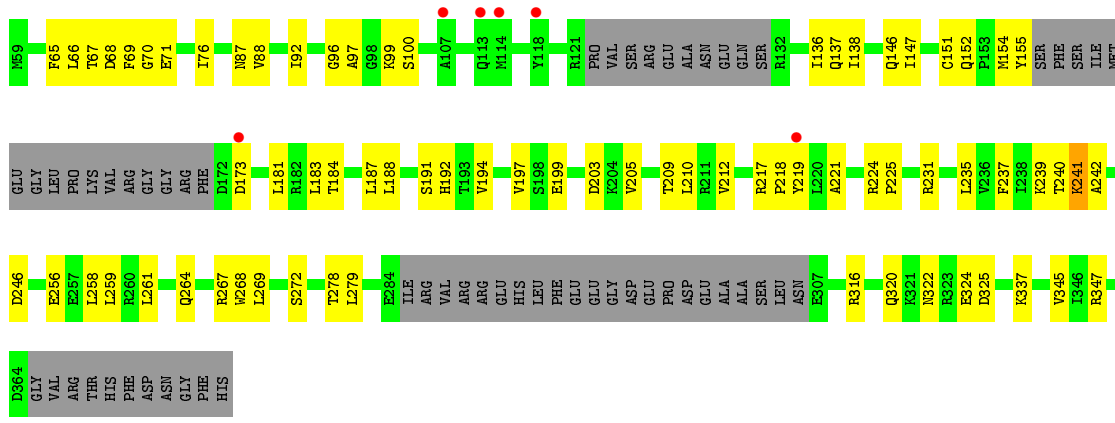




• Molecule 2: Protein smg-9

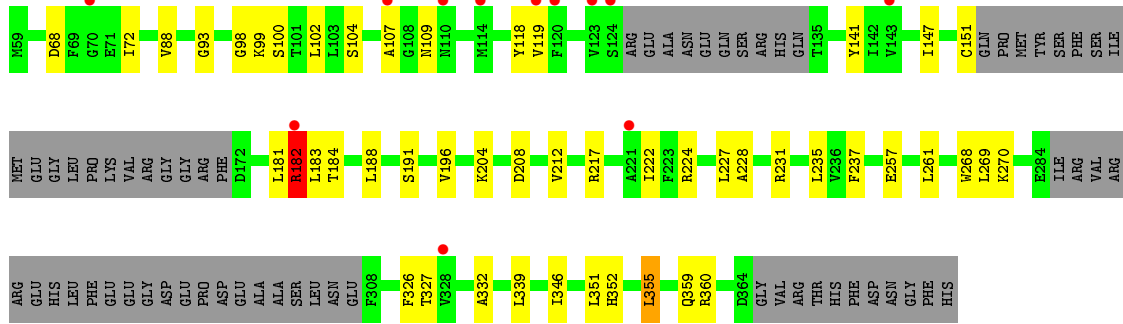


• Molecule 2: Protein smg-9



• Molecule 2: Protein smg-9





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.61Å 110.61Å 360.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.89 – 2.64 47.89 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.89-2.64) 99.8 (47.89-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.232 , 0.274 0.233 , 0.274	Depositor DCC
$R_{free}$ test set	3807 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtrriage
Anisotropy	0.514	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: GDP, MG, EDO, POP

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	0.25	0/2631	0.45	0/3558
1	C	0.26	0/2551	0.45	0/3454
1	E	0.26	0/2641	0.45	0/3580
2	B	0.26	0/1989	0.49	0/2701
2	D	0.25	0/2004	0.56	2/2721 (0.1%)
2	F	0.26	0/1898	0.53	1/2586 (0.0%)
All	All	0.26	0/13714	0.48	3/18600 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	241	LYS	CD-CE-NZ	-12.13	83.80	111.70
2	F	182	ARG	NE-CZ-NH2	-5.95	117.32	120.30
2	D	241	LYS	CA-CB-CG	5.32	125.11	113.40

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	2597	0	2477	38	0
1	C	2517	0	2388	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2608	0	2419	38	0
2	B	1960	0	1912	59	0
2	D	1975	0	1896	50	0
2	F	1872	0	1736	36	0
3	D	9	0	0	2	0
4	E	4	0	6	0	0
5	F	28	0	12	2	0
6	F	1	0	0	0	0
7	A	47	0	0	3	0
7	B	33	0	0	3	0
7	C	36	0	0	0	0
7	D	20	0	0	0	0
7	E	20	0	0	1	0
7	F	12	0	0	1	0
All	All	13739	0	12846	239	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 9.

All (239) 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:D:96:GLY:O	2:D:241:LYS:HE3	1.43	1.17
2:D:96:GLY:O	2:D:241:LYS:CE	2.18	0.90
2:F:182:ARG:HG3	2:F:355:LEU:HD13	1.56	0.87
2:F:182:ARG:HG3	2:F:355:LEU:CD1	2.05	0.86
1:C:42:ASN:ND2	1:C:50:PHE:H	1.82	0.78
2:B:191:SER:O	2:B:231:ARG:NH2	2.20	0.74
2:F:88:VAL:HG22	2:F:147:ILE:HB	1.73	0.71
1:A:37:LYS:HE2	1:A:78:ASN:HA	1.73	0.70
2:D:231:ARG:NH1	2:D:324:GLU:O	2.24	0.70
1:C:37:LYS:HE2	1:C:78:ASN:HA	1.72	0.70
2:B:141:TYR:CE2	2:B:143:VAL:HG13	2.27	0.69
1:E:242:LEU:HD23	1:E:248:VAL:HG11	1.72	0.69
1:A:37:LYS:O	7:A:501:HOH:O	2.10	0.69
2:B:211:ARG:NH1	2:B:214:GLU:OE1	2.26	0.68
1:C:41:ILE:O	1:C:45:LEU:HD12	1.94	0.68
1:E:37:LYS:HE2	1:E:78:ASN:HA	1.75	0.68
1:E:343:GLN:NE2	1:E:401:VAL:O	2.27	0.67
1:E:242:LEU:O	7:E:601:HOH:O	2.14	0.66
2:B:343:ARG:NH1	7:B:401:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:SER:O	2:F:231:ARG:NH2	2.28	0.66
2:B:234:ASN:HA	2:B:270:LYS:HG2	1.78	0.65
2:F:100:SER:N	5:F:401:GDP:O1B	2.22	0.65
2:F:151:CYS:N	7:F:501:HOH:O	2.30	0.64
1:C:7:VAL:HG11	1:C:316:ASN:HB2	1.80	0.64
2:B:144:ASN:OD1	2:B:145:HIS:N	2.27	0.63
1:C:42:ASN:HD21	1:C:50:PHE:H	1.45	0.63
1:A:7:VAL:HG11	1:A:316:ASN:HB2	1.81	0.63
1:C:25:ILE:HD12	1:C:122:PHE:HB2	1.80	0.63
1:E:25:ILE:HD12	1:E:122:PHE:HB2	1.80	0.63
2:F:107:ALA:HB1	2:F:141:TYR:CE1	2.34	0.63
2:B:61:GLU:OE1	2:B:121:ARG:NH2	2.32	0.62
2:B:141:TYR:HE2	2:B:143:VAL:HG13	1.64	0.61
2:F:98:GLY:HA3	5:F:401:GDP:HN22	1.66	0.61
1:E:22:ILE:HG22	1:E:71:GLN:HB3	1.82	0.61
1:C:35:HIS:CD2	1:C:39:ASP:HB2	2.35	0.61
2:F:182:ARG:HG3	2:F:355:LEU:HD11	1.82	0.60
2:F:351:LEU:O	2:F:355:LEU:HD23	2.01	0.60
2:B:99:LYS:NZ	2:B:151:CYS:O	2.30	0.59
1:E:311:VAL:O	1:E:315:MET:HG2	2.02	0.59
2:D:217:ARG:HD2	2:D:268:TRP:CZ3	2.37	0.59
2:B:239:LYS:NZ	7:B:404:HOH:O	2.33	0.59
2:D:66:LEU:HD13	2:D:70:GLY:HA2	1.84	0.59
2:F:72:ILE:HG21	2:F:339:LEU:HD11	1.85	0.58
1:A:17:GLN:NE2	1:A:68:GLU:OE2	2.35	0.58
1:E:41:ILE:HD11	1:E:50:PHE:CE2	2.38	0.57
2:D:181:LEU:HD21	2:D:212:VAL:HG12	1.86	0.57
2:B:327:THR:OG1	2:B:329:GLU:O	2.22	0.57
2:D:194:VAL:HG22	2:D:235:LEU:HD23	1.86	0.57
2:D:68:ASP:OD1	1:E:245:THR:HG22	2.04	0.57
2:B:88:VAL:HG22	2:B:147:ILE:HB	1.85	0.57
2:F:217:ARG:HD2	2:F:268:TRP:CZ3	2.40	0.57
1:A:311:VAL:O	1:A:315:MET:HG2	2.05	0.57
1:C:218:LEU:HB2	1:C:249:VAL:HG11	1.87	0.57
2:F:107:ALA:HB1	2:F:141:TYR:HE1	1.69	0.57
1:A:25:ILE:HD12	1:A:122:PHE:HB2	1.87	0.56
1:A:291:PHE:CZ	1:A:295:LEU:HD11	2.41	0.56
1:A:135:GLU:OE1	2:B:205:VAL:HG13	2.06	0.56
1:E:77:MET:HG3	1:E:112:MET:HE2	1.87	0.56
2:B:72:ILE:HG21	2:B:339:LEU:HD11	1.87	0.56
1:E:62:ILE:HG13	1:E:112:MET:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:LYS:NZ	2:B:208:ASP:OD2	2.38	0.56
2:B:253:ARG:HH11	2:B:253:ARG:HG3	1.69	0.56
1:E:91:LYS:HE2	2:F:261:LEU:HD21	1.88	0.56
1:E:18:LEU:HB3	1:E:309:GLU:HB2	1.88	0.55
2:B:239:LYS:HB3	2:B:281:VAL:HG22	1.89	0.55
2:B:256:GLU:O	2:B:260:ARG:HG3	2.06	0.55
1:C:42:ASN:HB3	1:C:47:GLU:O	2.07	0.55
2:B:59:MET:HE2	2:B:79:LEU:HG	1.88	0.55
2:D:137:GLN:NE2	2:D:138:ILE:O	2.40	0.54
1:A:87:ARG:O	1:A:91:LYS:HG2	2.07	0.54
2:B:136:ILE:HD13	2:B:182:ARG:HH12	1.72	0.54
2:B:76:ILE:HD11	2:B:339:LEU:HD13	1.89	0.54
1:A:75:LEU:HD22	7:A:542:HOH:O	2.07	0.54
2:F:327:THR:HG21	2:F:332:ALA:HB3	1.89	0.54
2:B:61:GLU:HA	2:B:119:VAL:HG23	1.89	0.54
2:B:240:THR:HB	2:B:241:LYS:HG3	1.89	0.54
2:B:255:ARG:NH1	7:B:405:HOH:O	2.41	0.54
1:A:221:GLN:O	1:A:225:ILE:HD12	2.08	0.53
2:F:119:VAL:HG21	2:F:141:TYR:CD2	2.44	0.53
2:D:188:LEU:HD13	2:D:269:LEU:HD21	1.90	0.53
2:B:217:ARG:HD2	2:B:268:TRP:CZ3	2.44	0.52
2:D:205:VAL:O	2:D:209:THR:HG23	2.08	0.52
2:B:67:THR:OG1	2:B:68:ASP:N	2.42	0.52
1:C:170:ASN:OD1	1:C:170:ASN:N	2.43	0.52
2:D:218:PRO:HG3	2:D:345:VAL:HG23	1.92	0.52
1:C:242:LEU:HD22	1:C:248:VAL:HG11	1.90	0.52
1:A:396:ASP:O	2:B:267:ARG:NH2	2.42	0.52
2:F:184:THR:O	2:F:188:LEU:HG	2.10	0.52
2:D:66:LEU:HB2	2:D:137:GLN:OE1	2.09	0.51
1:A:96:SER:OG	1:A:97:ASN:N	2.43	0.51
2:B:253:ARG:HD2	2:B:253:ARG:O	2.11	0.51
2:D:191:SER:O	2:D:231:ARG:NH2	2.43	0.51
2:F:222:ILE:HA	2:F:224:ARG:HH11	1.75	0.51
1:A:246:ILE:HG13	1:A:247:PRO:HD2	1.93	0.51
2:B:89:ILE:HD13	2:B:319:LEU:HD13	1.92	0.51
2:D:151:CYS:SG	2:D:152:GLN:N	2.84	0.51
1:E:96:SER:OG	1:E:97:ASN:N	2.44	0.51
1:A:410:LEU:HA	1:A:413:GLN:HG3	1.92	0.50
2:B:106:LEU:HD22	2:B:319:LEU:HD11	1.93	0.50
2:F:109:ASN:ND2	2:F:118:TYR:HA	2.26	0.50
2:F:188:LEU:HD13	2:F:269:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:ARG:HA	2:D:225:PRO:C	2.32	0.50
2:D:65:PHE:N	2:D:137:GLN:HE22	2.09	0.50
1:E:410:LEU:HA	1:E:413:GLN:HG2	1.93	0.50
1:A:170:ASN:N	1:A:170:ASN:OD1	2.43	0.50
1:A:134:LEU:O	1:A:138:ARG:HG3	2.12	0.49
1:A:170:ASN:OD1	7:A:502:HOH:O	2.19	0.49
2:B:70:GLY:HA2	2:B:136:ILE:HD11	1.93	0.49
1:E:245:THR:HG23	1:E:246:ILE:HG13	1.94	0.49
2:D:151:CYS:HB2	2:D:187:LEU:HD11	1.94	0.49
1:C:311:VAL:O	1:C:315:MET:HG2	2.12	0.49
2:B:106:LEU:HG	2:B:312:ILE:HG23	1.93	0.49
2:D:316:ARG:O	2:D:320:GLN:NE2	2.44	0.49
1:C:30:LYS:HB2	1:C:32:TYR:HE2	1.78	0.49
1:E:113:LEU:HB2	1:E:143:VAL:HG21	1.93	0.49
1:C:220:ASN:OD1	1:C:220:ASN:N	2.46	0.48
2:F:352:HIS:HA	2:F:355:LEU:HD21	1.95	0.48
1:E:77:MET:HG3	1:E:112:MET:CE	2.43	0.48
1:A:246:ILE:HG22	2:F:68:ASP:OD2	2.14	0.48
2:B:315:LEU:O	2:B:319:LEU:HG	2.14	0.48
2:D:136:ILE:HB	2:D:183:LEU:HD11	1.95	0.47
2:B:232:LYS:HB3	2:B:270:LYS:HB3	1.95	0.47
2:B:256:GLU:HA	2:B:259:LEU:HD12	1.96	0.47
2:F:257:GLU:O	2:F:261:LEU:HD12	2.15	0.47
1:A:291:PHE:O	1:A:295:LEU:HD12	2.15	0.47
1:A:170:ASN:OD1	1:A:171:ARG:N	2.48	0.47
1:E:227:LYS:HG2	1:E:232:ILE:HD11	1.97	0.47
1:C:80:VAL:HG11	1:C:106:GLU:HA	1.97	0.46
2:D:92:ILE:HD11	2:D:210:LEU:HD21	1.96	0.46
2:D:99:LYS:NZ	3:D:401:POP:O6	2.49	0.46
1:E:394:TYR:O	1:E:398:VAL:HG22	2.14	0.46
1:E:169:ASN:HD21	1:E:171:ARG:NH2	2.13	0.46
2:B:235:LEU:HD11	2:B:269:LEU:HB3	1.97	0.46
1:A:63:ARG:HB2	1:A:76:VAL:HG22	1.98	0.46
2:D:71:GLU:OE2	1:E:170:ASN:ND2	2.49	0.46
1:A:42:ASN:HB2	1:A:48:ASN:HA	1.97	0.46
2:D:242:ALA:HB1	2:D:246:ASP:HB2	1.98	0.46
2:D:347:ARG:NH1	1:E:305:GLU:OE1	2.49	0.46
1:E:22:ILE:HD11	1:E:311:VAL:HG21	1.97	0.46
1:E:23:LYS:NZ	1:E:302:GLU:O	2.40	0.46
2:D:100:SER:OG	3:D:401:POP:O6	2.34	0.46
1:C:35:HIS:HD2	1:C:36:GLY:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:228:ALA:N	2:F:326:PHE:O	2.33	0.45
2:F:352:HIS:HA	2:F:355:LEU:CD2	2.46	0.45
2:D:347:ARG:HD2	1:E:305:GLU:OE2	2.17	0.45
2:D:256:GLU:HA	2:D:259:LEU:HD12	1.98	0.45
1:E:107:CYS:O	1:E:111:ARG:HG3	2.17	0.45
2:F:227:LEU:HA	2:F:327:THR:HA	1.97	0.45
2:B:71:GLU:HB2	1:C:170:ASN:HD21	1.81	0.45
1:C:83:VAL:HG13	2:D:258:LEU:HD11	1.98	0.45
2:D:67:THR:OG1	2:D:68:ASP:N	2.47	0.45
1:E:308:LEU:O	1:E:312:ILE:HG13	2.17	0.45
1:E:44:TYR:HD1	1:E:292:VAL:HG23	1.82	0.45
1:C:169:ASN:HD21	1:C:171:ARG:NH2	2.15	0.44
2:F:196:VAL:HG21	2:F:237:PHE:CD2	2.53	0.44
2:B:142:ILE:HA	2:B:146:GLN:O	2.18	0.44
1:E:243:ASN:ND2	1:E:298:ASN:OD1	2.50	0.44
2:F:182:ARG:NH2	2:F:346:ILE:HG23	2.33	0.44
1:C:138:ARG:O	1:C:142:LYS:HG3	2.17	0.44
2:F:93:GLY:O	2:F:99:LYS:NZ	2.51	0.44
1:A:170:ASN:OD1	1:A:171:ARG:HG3	2.18	0.44
1:C:42:ASN:OD1	1:C:50:PHE:CD1	2.71	0.44
2:F:181:LEU:HD21	2:F:212:VAL:HG12	1.99	0.44
2:F:235:LEU:HD11	2:F:269:LEU:HB3	1.99	0.44
1:A:74:PHE:O	1:A:75:LEU:HD23	2.18	0.44
2:B:70:GLY:CA	2:B:136:ILE:HD11	2.48	0.44
1:C:16:THR:HG22	1:C:17:GLN:OE1	2.17	0.44
2:D:219:TYR:CE2	2:D:221:ALA:HB2	2.53	0.44
1:E:75:LEU:HD11	1:E:315:MET:HE1	2.00	0.44
1:C:138:ARG:NH1	2:D:173:ASP:OD1	2.51	0.44
1:A:122:PHE:CD2	1:A:186:ARG:HB2	2.53	0.43
1:A:338:PHE:O	1:A:342:ILE:HG13	2.18	0.43
2:B:352:HIS:CE1	1:C:172:ILE:HG12	2.53	0.43
1:C:400:GLY:HA2	2:D:267:ARG:HD3	2.00	0.43
2:F:151:CYS:SG	2:F:183:LEU:HD21	2.58	0.43
2:B:119:VAL:HG21	2:B:141:TYR:CE1	2.52	0.43
1:C:30:LYS:NZ	1:C:81:ASP:OD1	2.51	0.43
2:D:88:VAL:HG22	2:D:147:ILE:HB	1.99	0.43
1:E:3:ILE:HG12	1:E:315:MET:HE3	2.01	0.43
2:D:192:HIS:HA	2:D:231:ARG:HH22	1.83	0.43
2:D:203:ASP:OD1	2:D:205:VAL:HG12	2.19	0.43
2:B:198:SER:HB3	2:B:201:HIS:CE1	2.53	0.43
2:D:272:SER:OG	2:D:278:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:ALA:HB1	1:E:252:LEU:HD11	2.00	0.43
2:B:193:THR:HG22	2:B:234:ASN:HB3	2.00	0.42
2:F:204:LYS:NZ	2:F:208:ASP:OD1	2.43	0.42
1:C:27:VAL:HB	1:C:76:VAL:HG22	2.01	0.42
2:D:65:PHE:HA	2:D:76:ILE:HD11	2.01	0.42
1:E:306:ILE:HD13	1:E:311:VAL:HG12	2.00	0.42
2:D:67:THR:N	2:D:71:GLU:O	2.42	0.42
2:D:97:ALA:HB1	2:D:197:VAL:HG12	2.00	0.42
1:C:45:LEU:CD2	1:C:65:HIS:HE1	2.31	0.42
1:C:75:LEU:HD11	1:C:315:MET:HE1	2.01	0.42
2:F:196:VAL:HG22	2:F:237:PHE:HA	2.00	0.42
1:A:342:ILE:HG21	2:B:354:THR:HG23	2.02	0.42
2:B:229:ILE:HA	2:B:229:ILE:HD13	1.89	0.42
1:A:136:LEU:O	1:A:140:LEU:HG	2.20	0.42
2:B:80:LEU:HB3	2:B:335:GLU:HG3	2.02	0.42
2:B:88:VAL:HG21	2:B:338:TRP:CE2	2.55	0.42
2:D:184:THR:O	2:D:188:LEU:HG	2.19	0.42
1:A:158:LEU:HD21	1:A:318:LEU:HD21	2.02	0.42
2:B:184:THR:O	2:B:188:LEU:HG	2.20	0.42
2:B:92:ILE:HD11	2:B:210:LEU:HD21	2.01	0.42
1:C:350:ALA:HB1	1:C:391:ALA:HB1	2.02	0.42
2:B:140:ILE:HG13	2:B:141:TYR:N	2.35	0.41
1:E:16:THR:HG22	1:E:17:GLN:OE1	2.19	0.41
1:A:107:CYS:O	1:A:111:ARG:HG3	2.20	0.41
1:C:35:HIS:CD2	1:C:36:GLY:O	2.72	0.41
1:C:87:ARG:O	1:C:91:LYS:HG3	2.20	0.41
2:D:199:GLU:HG2	2:D:240:THR:HG23	2.02	0.41
1:C:68:GLU:H	1:C:68:GLU:HG2	1.62	0.41
2:D:261:LEU:HD12	2:D:264:GLN:OE1	2.20	0.41
2:D:239:LYS:HB2	2:D:279:LEU:HD11	2.01	0.41
1:E:163:LEU:HD23	1:E:166:VAL:HG21	2.02	0.41
2:F:119:VAL:HG21	2:F:141:TYR:CE2	2.55	0.41
1:A:113:LEU:HB2	1:A:143:VAL:HG21	2.03	0.41
2:B:335:GLU:O	2:B:338:TRP:HB3	2.21	0.41
2:F:104:SER:O	2:F:107:ALA:HB3	2.20	0.41
1:A:135:GLU:HB2	1:A:138:ARG:NH1	2.36	0.41
1:A:30:LYS:HE2	1:A:81:ASP:OD2	2.20	0.41
1:A:90:LEU:O	2:B:264:GLN:NE2	2.51	0.41
2:D:235:LEU:HD11	2:D:269:LEU:HB3	2.02	0.41
2:B:267:ARG:HG2	2:B:268:TRP:CE2	2.56	0.41
2:D:237:PHE:O	2:D:279:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:PHE:CG	1:E:171:ARG:HD3	2.56	0.41
1:A:403:SER:OG	2:B:267:ARG:NH1	2.54	0.41
2:B:95:GLN:HA	2:B:153:PRO:HB3	2.02	0.41
2:B:136:ILE:CD1	2:B:182:ARG:HH12	2.34	0.41
2:B:140:ILE:HD11	2:B:147:ILE:HG23	2.03	0.41
2:B:253:ARG:NH1	2:B:253:ARG:HG3	2.35	0.41
2:D:97:ALA:O	2:D:240:THR:HG21	2.21	0.41
2:D:87:ASN:HB3	2:D:146:GLN:OE1	2.21	0.41
1:A:49:VAL:HG11	1:A:65:HIS:CG	2.56	0.40
1:C:113:LEU:HB2	1:C:143:VAL:HG21	2.04	0.40
1:C:308:LEU:O	1:C:312:ILE:HG13	2.21	0.40
1:E:151:ARG:HG3	1:E:179:GLU:CD	2.41	0.40
1:A:77:MET:HE1	1:A:109:GLN:HG3	2.03	0.40
2:B:151:CYS:HB2	2:B:187:LEU:HD11	2.03	0.40
2:D:347:ARG:O	2:D:347:ARG:HG2	2.21	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	332/429 (77%)	320 (96%)	12 (4%)	0	100	100
1	C	322/429 (75%)	309 (96%)	13 (4%)	0	100	100
1	E	339/429 (79%)	326 (96%)	13 (4%)	0	100	100
2	B	248/317 (78%)	238 (96%)	10 (4%)	0	100	100
2	D	250/317 (79%)	239 (96%)	11 (4%)	0	100	100
2	F	245/317 (77%)	233 (95%)	12 (5%)	0	100	100
All	All	1736/2238 (78%)	1665 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	275/391 (70%)	271 (98%)	4 (2%)	65	79
1	C	267/391 (68%)	264 (99%)	3 (1%)	73	85
1	E	269/391 (69%)	263 (98%)	6 (2%)	52	70
2	B	205/288 (71%)	203 (99%)	2 (1%)	76	86
2	D	205/288 (71%)	200 (98%)	5 (2%)	49	67
2	F	185/288 (64%)	179 (97%)	6 (3%)	39	56
All	All	1406/2037 (69%)	1380 (98%)	26 (2%)	59	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	137	MET
1	A	168	PHE
1	A	193	ARG
2	B	85	ASN
2	B	337	LYS
1	C	15	SER
1	C	67	SER
1	C	114	HIS
2	D	154	MET
2	D	155	TYR
2	D	322	ASN
2	D	325	ASP
2	D	337	LYS
1	E	15	SER
1	E	114	HIS
1	E	168	PHE
1	E	253	ASN
1	E	385	LEU
1	E	410	LEU
2	F	102	LEU
2	F	182	ARG

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Mol	Chain	Res	Type
2	F	270	LYS
2	F	355	LEU
2	F	359	GLN
2	F	360	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	C	35	HIS
1	C	42	ASN
1	C	65	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z  > 2$
5	GDP	F	401	6	24,30,30	1.19	2 (8%)	31,47,47	2.01	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	POP	D	401	-	6,8,8	0.73	0	13,13,13	1.19	1 (7%)
4	EDO	E	501	-	3,3,3	0.46	0	2,2,2	0.32	0

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
5	GDP	F	401	6	-	5/12/32/32	0/3/3/3
3	POP	D	401	-	-	0/6/6/6	-
4	EDO	E	501	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	401	GDP	C6-C5	4.17	1.48	1.41
5	F	401	GDP	C5-C4	2.49	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	401	GDP	C2-N3-C4	4.91	120.97	115.36
5	F	401	GDP	C6-N1-C2	3.98	122.26	115.93
5	F	401	GDP	C5-C6-N1	-3.98	117.98	123.43
5	F	401	GDP	PA-O3A-PB	-3.74	120.01	132.83
5	F	401	GDP	C6-C5-C4	-3.62	117.34	120.80
5	F	401	GDP	N3-C2-N1	-3.21	122.95	127.22
5	F	401	GDP	C3'-C2'-C1'	3.03	105.55	100.98
3	D	401	POP	P2-O-P1	-2.87	122.98	132.83
5	F	401	GDP	C4-C5-N7	-2.61	106.67	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

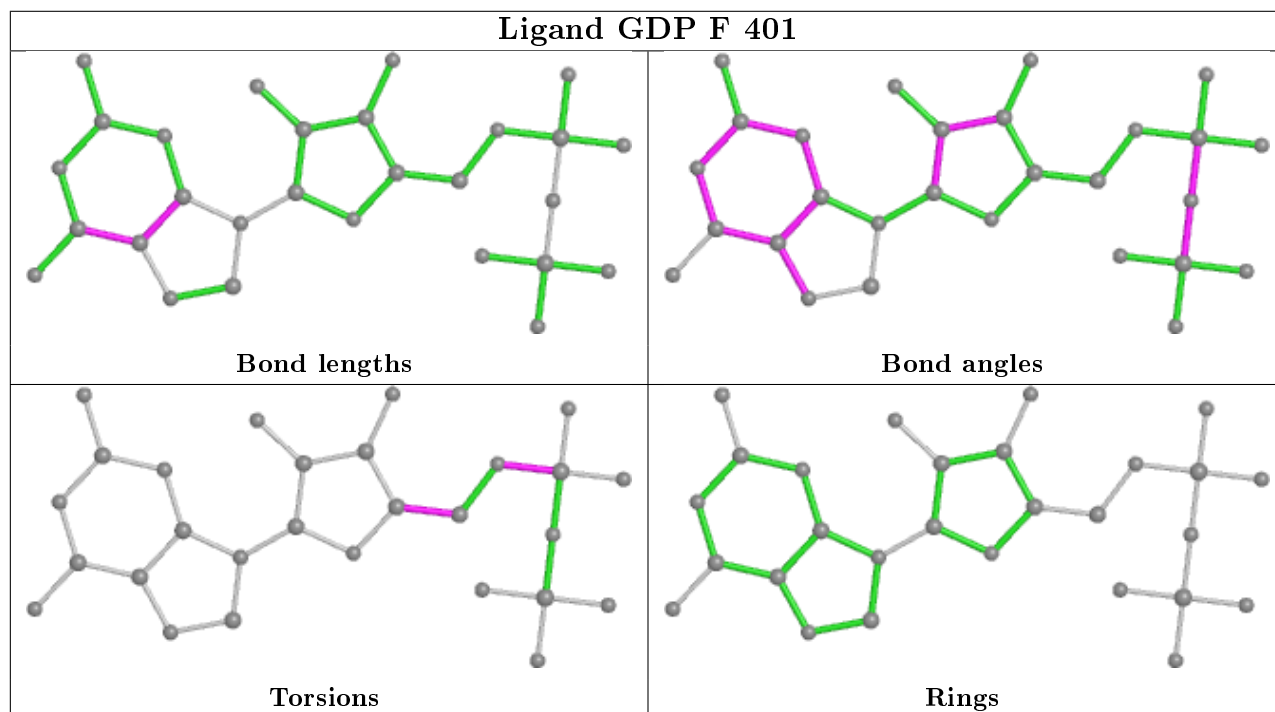
Mol	Chain	Res	Type	Atoms
5	F	401	GDP	C5'-O5'-PA-O3A
5	F	401	GDP	C5'-O5'-PA-O2A
5	F	401	GDP	O4'-C4'-C5'-O5'
5	F	401	GDP	C3'-C4'-C5'-O5'
5	F	401	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	401	GDP	2	0
3	D	401	POP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

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 [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, 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	A	340/429 (79%)	-0.04	8 (2%) 59 55	46, 72, 126, 146	0
1	C	330/429 (76%)	0.10	13 (3%) 39 36	48, 74, 123, 167	0
1	E	347/429 (80%)	-0.02	9 (2%) 56 52	49, 76, 134, 187	0
2	B	256/317 (80%)	0.17	6 (2%) 60 57	50, 81, 121, 156	0
2	D	258/317 (81%)	0.14	6 (2%) 60 57	50, 83, 124, 159	0
2	F	253/317 (79%)	0.12	12 (4%) 31 27	52, 88, 129, 147	0
All	All	1784/2238 (79%)	0.07	54 (3%) 50 46	46, 78, 128, 187	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	CYS	7.0
1	A	214	LEU	5.2
1	C	412	ALA	5.1
1	E	412	ALA	4.8
1	E	418	TRP	4.6
1	E	384	HIS	3.9
1	A	417	MET	3.6
2	D	114	MET	3.4
1	E	414	CYS	3.2
2	B	308	PHE	3.2
1	C	391	ALA	3.2
2	B	222	ILE	3.1
2	F	328	VAL	3.1
1	C	413	GLN	3.0
1	C	417	MET	3.0
1	C	408	SER	2.9
2	F	221	ALA	2.9
2	D	107	ALA	2.9
2	F	110	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	412	ALA	2.8
1	C	394	TYR	2.7
2	D	118	TYR	2.7
2	B	144	ASN	2.6
2	F	114	MET	2.6
1	C	326	LEU	2.6
2	F	124	SER	2.6
1	A	395	ILE	2.6
2	D	219	TYR	2.6
1	C	410	LEU	2.5
2	B	109	ASN	2.5
2	F	143	VAL	2.4
1	C	415	ASN	2.4
2	F	123	VAL	2.4
1	E	351	ARG	2.3
2	D	113	GLN	2.3
2	F	70	GLY	2.3
2	F	182	ARG	2.3
1	A	95	LYS	2.3
1	C	416	GLU	2.3
2	B	112	ARG	2.3
1	C	392	THR	2.3
1	A	394	TYR	2.3
1	A	350	ALA	2.2
2	F	119	VAL	2.2
2	F	120	PHE	2.2
1	E	159	VAL	2.2
1	C	411	GLN	2.2
2	D	173	ASP	2.1
1	A	347	MET	2.1
2	B	312	ILE	2.1
1	E	353	LEU	2.1
1	E	413	GLN	2.0
2	F	107	ALA	2.0
1	E	408	SER	2.0

## 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 [i](#)

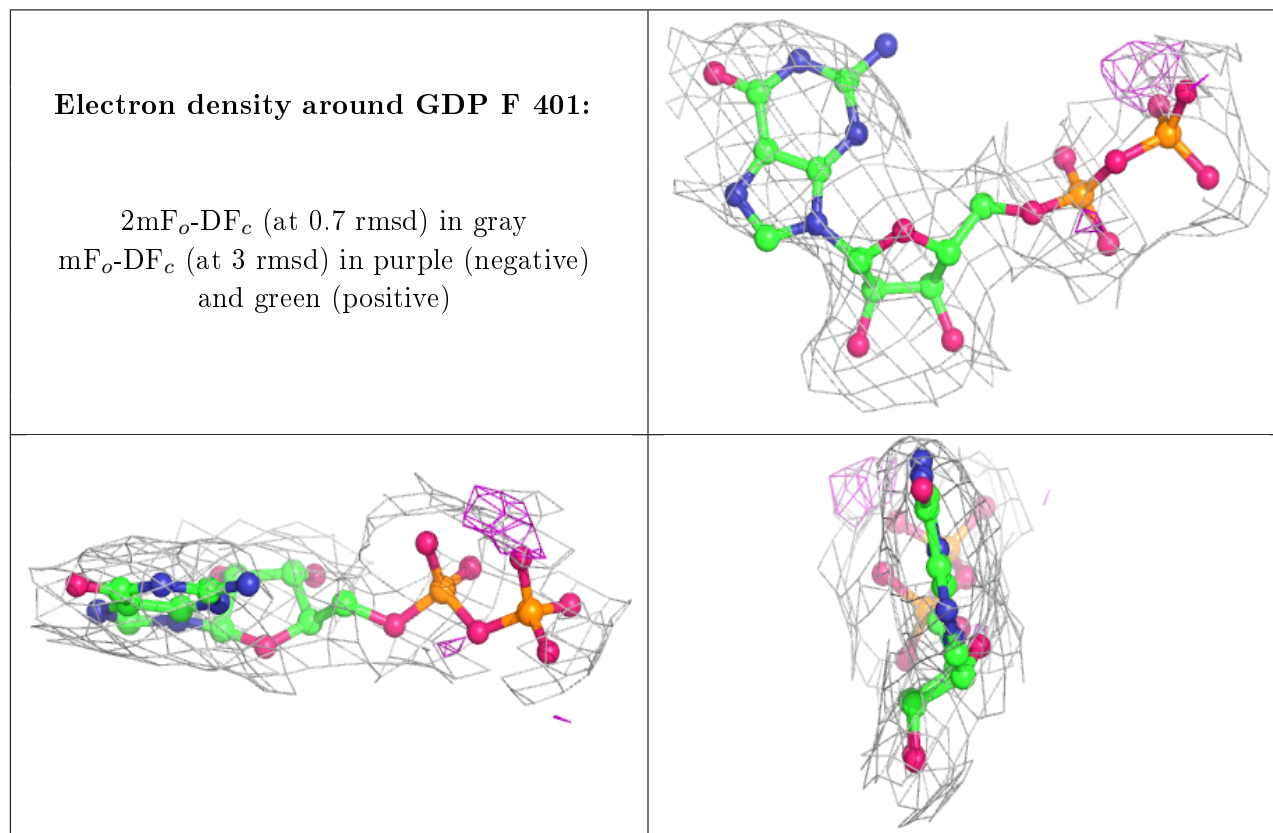
There are no monosaccharides in this entry.

### 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	POP	D	401	9/9	0.60	0.26	186,188,189,191	0
4	EDO	E	501	4/4	0.61	0.19	95,97,97,98	0
5	GDP	F	401	28/28	0.88	0.17	94,110,113,116	0
6	MG	F	402	1/1	0.95	0.14	100,100,100,100	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.