



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 01:08 PM GMT

PDB ID : 7AIG
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEX WITH DNA AND L-GLUTAMATE TENOFOVIR
Authors : Gu, W.; Martinez, S.E.; Nguyen, H.; Xu, H.; Herdewijn, P.; de Jonghe, S.; Das, K.
Deposited on : 2020-09-27
Resolution : 2.95 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

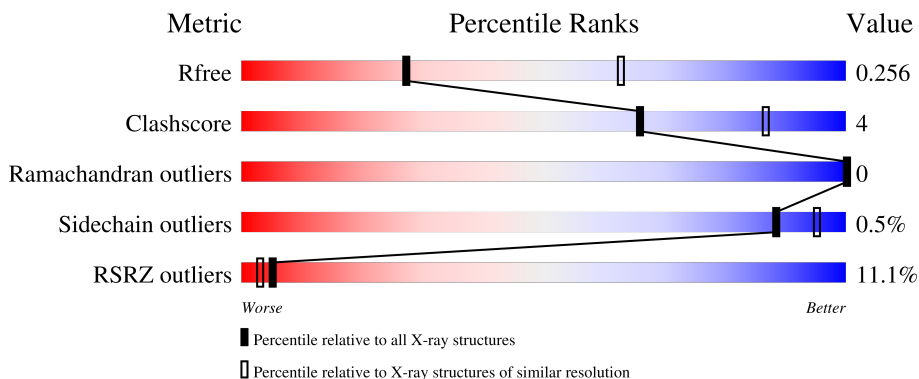
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	A	556	 17% 88% 12%
1	C	556	 15% 89% 11%
2	B	428	 3% 86% 10% .
2	D	428	 7% 85% 11% .
3	E	27	 11% 59% 30% 1%

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Mol	Chain	Length	Quality of chain
3	T	27	
4	F	21	
4	P	21	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17692 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 Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	Total	C	N	O	S	0	0	0
			4513	2922	751	832	8			
1	C	556	Total	C	N	O	S	0	0	0
			4521	2927	752	833	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	258	CYS	GLN	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	411	Total	C	N	O	S	0	0	0
			3401	2215	563	616	7			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

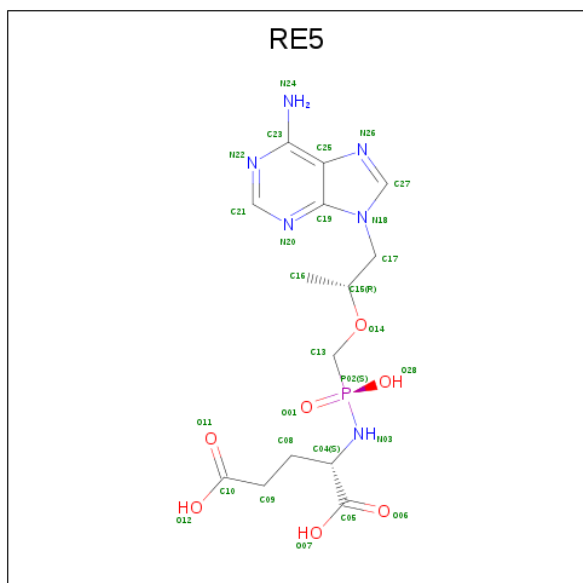
- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	23	Total	C	N	O	P	0	0	0
			477	223	95	136	23			
3	E	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(DDG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	20	Total	C	N	O	P	0	0	0
			403	192	72	120	19			
4	F	20	Total	C	N	O	P	0	0	0
			403	192	72	120	19			

- Molecule 5 is L-Glutamate Tenofovir (three-letter code: RE5) (formula: C₁₄H₂₁N₆O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			28	14	6	7	1		

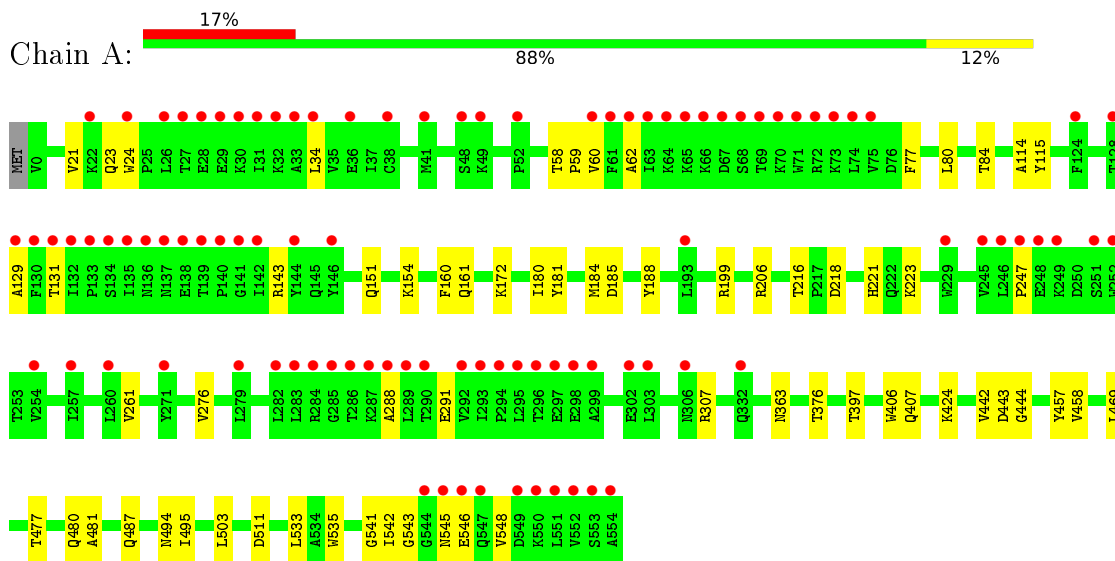
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	14	Total O 14 14	0	0
6	C	12	Total O 12 12	0	0
6	D	7	Total O 7 7	0	0
6	T	1	Total O 1 1	0	0
6	P	1	Total O 1 1	0	0
6	E	5	Total O 5 5	0	0

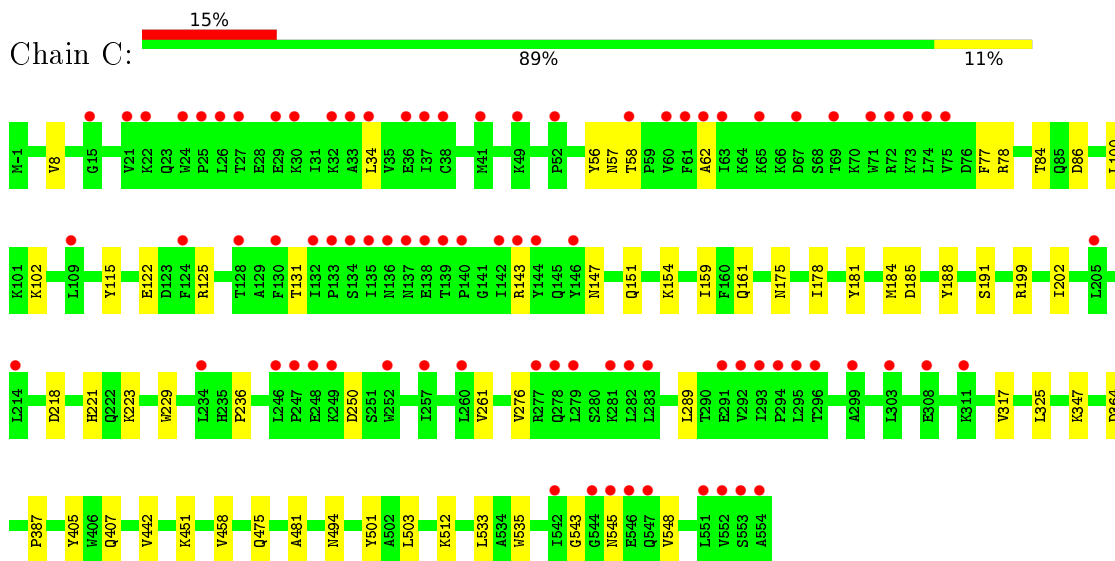
3 Residue-property plots

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: Gag-Pol polyprotein



- Molecule 1: Gag-Pol polyprotein



- Molecule 2: Gag-Pol polyprotein

- Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(DDG))-3')

Chain F:  67% 29% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.70Å 133.55Å 140.43Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	54.00 – 2.95 54.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (54.00-2.95) 99.4 (54.00-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.96Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.213 , 0.257 0.213 , 0.256	Depositor DCC
R_{free} test set	2085 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17692	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MRG, DDG, RE5

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/4631	0.40	0/6293
1	C	0.23	0/4639	0.40	0/6303
2	B	0.23	0/3499	0.40	0/4752
2	D	0.23	0/3497	0.41	0/4751
3	E	0.49	0/555	0.80	0/856
3	T	0.49	0/536	0.78	0/826
4	F	0.55	0/400	0.91	0/612
4	P	0.52	0/400	0.89	0/612
All	All	0.27	0/18157	0.47	0/25005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4513	0	4578	40	0
1	C	4521	0	4587	37	0
2	B	3401	0	3431	28	0
2	D	3400	0	3433	25	0
3	E	494	0	269	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	477	0	256	6	0
4	F	403	0	224	7	0
4	P	403	0	224	4	0
5	C	28	0	0	0	0
6	A	12	0	0	1	0
6	B	14	0	0	0	0
6	C	12	0	0	0	0
6	D	7	0	0	0	0
6	E	5	0	0	0	0
6	P	1	0	0	0	0
6	T	1	0	0	0	0
All	All	17692	0	17002	138	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 4.

All (138) 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:B:125:ARG:HE	2:B:147:ASN:HA	1.57	0.69
1:C:56:TYR:O	1:C:143:ARG:NH2	2.26	0.68
1:C:543:GLY:N	2:D:283:LEU:O	2.25	0.67
1:A:543:GLY:N	2:B:283:LEU:O	2.27	0.67
1:C:178:ILE:HG13	1:C:191:SER:HB3	1.78	0.65
2:D:359:GLY:O	2:D:367:GLN:NE2	2.30	0.65
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.81	0.63
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.79	0.62
1:A:199:ARG:HH12	1:A:223:LYS:HB3	1.64	0.62
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.33	0.60
1:A:206:ARG:NH2	1:A:216:THR:O	2.33	0.60
2:B:122:GLU:OE1	2:B:125:ARG:NH1	2.34	0.60
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.85	0.59
1:C:125:ARG:HE	1:C:147:ASN:HA	1.68	0.59
1:A:172:LYS:HE2	1:A:180:ILE:HB	1.85	0.59
1:C:199:ARG:HA	1:C:202:ILE:HD12	1.85	0.59
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.84	0.58
2:B:358:ARG:NH2	2:B:405:TYR:O	2.36	0.58
1:C:102:LYS:NZ	1:C:236:PRO:O	2.33	0.58
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.86	0.57
1:A:115:TYR:HD2	1:A:151:GLN:HG2	1.68	0.57
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.86	0.56
1:C:364:ASP:OD1	1:C:512:LYS:NZ	2.31	0.56
1:C:451:LYS:NZ	4:F:808:DC:OP1	2.38	0.56
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.87	0.55
1:C:122:GLU:OE1	1:C:125:ARG:NH1	2.40	0.55
1:A:84:THR:HB	1:A:154:LYS:HE2	1.89	0.55
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.89	0.55
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.90	0.54
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.89	0.54
3:E:724:DT:H3	4:F:804:DA:H61	1.57	0.53
2:D:125:ARG:NH1	2:D:147:ASN:O	2.42	0.53
1:A:184:MET:HG3	4:P:822:DDG:H1'	1.91	0.53
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.90	0.52
2:D:73:LYS:NZ	2:D:146:TYR:OH	2.38	0.52
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.92	0.52
1:C:218:ASP:HA	1:C:221:HIS:HB2	1.92	0.52
4:F:818:DC:H2'	4:F:819:DG:H8	1.75	0.51
1:C:84:THR:HB	1:C:154:LYS:HE2	1.93	0.51
3:E:718:DA:H1'	3:E:719:DG:C8	2.46	0.51
2:B:60:VAL:HG22	2:B:75:VAL:HG22	1.93	0.49
2:D:244:ILE:HD12	2:D:271:TYR:HE1	1.76	0.49
1:A:24:TRP:HD1	1:A:59:PRO:HB3	1.78	0.49
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.78	0.49
1:C:78:ARG:HD2	3:E:705:DT:H5''	1.95	0.49
3:T:709:DC:H2'	3:T:710:DG:C8	2.46	0.49
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.93	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.93	0.49
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.95	0.49
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.93	0.48
1:C:57:ASN:HD21	1:C:131:THR:HG22	1.77	0.48
2:D:91:GLN:HG2	2:D:92:LEU:HG	1.95	0.48
4:F:818:DC:H2'	4:F:819:DG:C8	2.48	0.48
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.48	0.48
2:B:320:ASP:O	2:B:343:GLN:NE2	2.43	0.47
1:A:218:ASP:HA	1:A:221:HIS:HB2	1.96	0.47
1:C:115:TYR:HD2	1:C:151:GLN:HG2	1.79	0.47
1:C:199:ARG:HH12	1:C:223:LYS:HB3	1.80	0.47
1:C:317:VAL:HG11	1:C:347:LYS:HB3	1.97	0.47
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.96	0.47
1:C:161:GLN:NE2	1:C:184:MET:SD	2.87	0.46
2:D:193:LEU:HB3	2:D:197:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:ASP:OD1	2:D:185:ASP:N	2.48	0.46
2:D:191:SER:OG	2:D:198:HIS:ND1	2.37	0.46
3:E:711:DC:H2'	3:E:712:DC:C6	2.51	0.46
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.97	0.46
2:D:138:GLU:HG2	2:D:139:THR:HG23	1.96	0.46
3:T:709:DC:H2'	3:T:710:DG:H8	1.81	0.46
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.97	0.46
2:D:287:LYS:HD3	2:D:293:ILE:HD11	1.98	0.46
4:P:818:DC:H2'	4:P:819:DG:C8	2.50	0.46
2:D:28:GLU:HG2	2:D:32:LYS:HE2	1.96	0.46
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.98	0.45
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.52	0.45
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.99	0.45
2:D:126:LYS:HE3	2:D:127:TYR:CZ	2.52	0.45
3:T:711:DC:H2'	3:T:712:DC:C6	2.51	0.45
1:A:406:TRP:CD1	1:A:407:GLN:HG2	2.51	0.45
1:A:58:THR:HG21	1:A:77:PHE:CE1	2.52	0.44
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.99	0.44
2:B:282:LEU:HD21	2:B:295:LEU:HA	1.99	0.44
1:C:545:ASN:HA	1:C:548:VAL:HG12	2.00	0.44
4:P:818:DC:H2'	4:P:819:DG:H8	1.82	0.44
3:T:703:DG:H21	3:T:705:DT:H73	1.82	0.44
1:C:503:LEU:HD12	1:C:533:LEU:HD13	2.00	0.44
1:C:58:THR:HG21	1:C:77:PHE:CD1	2.53	0.44
4:F:817:MRG:H2'	4:F:818:DC:C6	2.53	0.44
1:A:443:ASP:OD1	1:A:444:GLY:N	2.48	0.43
2:D:365:VAL:HG11	2:D:401:TRP:HB2	2.00	0.43
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.99	0.43
1:A:161:GLN:NE2	1:A:184:MET:SD	2.85	0.43
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.52	0.43
1:C:458:VAL:HG12	2:D:286:THR:HG21	2.00	0.43
3:T:714:DG:H2''	3:T:715:DA:C8	2.54	0.43
1:A:34:LEU:HD21	1:A:62:ALA:HB2	2.00	0.43
1:A:80:LEU:O	1:A:84:THR:OG1	2.28	0.43
2:B:154:LYS:HG2	2:B:184:MET:SD	2.58	0.43
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.53	0.43
4:P:817:MRG:H2'	4:P:818:DC:C6	2.54	0.43
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.54	0.42
2:D:21:VAL:HB	2:D:59:PRO:HD3	2.01	0.42
1:A:23:GLN:NE2	1:A:60:VAL:O	2.48	0.42
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:ARG:HD2	2:D:360:ALA:HB1	2.00	0.42
1:A:487:GLN:NE2	6:A:603:HOH:O	2.51	0.42
2:D:17:ASP:O	2:D:83:ARG:HD3	2.19	0.42
3:E:706:DC:H2'	3:E:707:DG:C8	2.54	0.42
1:A:247:PRO:O	1:A:307:ARG:NH2	2.52	0.42
1:A:58:THR:HG22	1:A:129:ALA:O	2.19	0.42
2:B:229:TRP:CG	2:B:230:MET:N	2.88	0.42
1:C:185:ASP:OD1	1:C:185:ASP:N	2.36	0.42
1:C:325:LEU:HB3	1:C:387:PRO:HB3	2.02	0.42
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.54	0.42
2:D:100:LEU:HG	2:D:381:VAL:HG13	2.01	0.42
2:B:17:ASP:O	2:B:83:ARG:HD3	2.19	0.41
1:C:8:VAL:HG21	1:C:159:ILE:HG23	2.02	0.41
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.01	0.41
2:B:178:ILE:HG12	2:B:191:SER:HB3	2.02	0.41
1:A:397:THR:HG21	1:A:424:LYS:HA	2.03	0.41
2:B:422:LEU:HG	2:B:422:LEU:H	1.50	0.41
1:C:175:ASN:O	1:C:178:ILE:HG22	2.20	0.41
1:C:86:ASP:O	2:D:55:PRO:HB3	2.21	0.41
2:B:191:SER:OG	2:B:198:HIS:ND1	2.47	0.41
2:B:276:VAL:H	2:B:277:ARG:HE	1.68	0.41
2:D:421:PRO:HB2	2:D:423:VAL:HG22	2.02	0.41
1:C:289:LEU:HD11	4:F:817:MRG:H4'	2.03	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.21	0.41
1:A:469:LEU:HD11	1:A:480:GLN:HG2	2.03	0.41
1:A:541:GLY:HA2	1:A:546:GLU:HB2	2.03	0.41
3:T:713:DC:H2'	3:T:714:DG:C8	2.56	0.41
1:C:250:ASP:N	1:C:250:ASP:OD1	2.54	0.40
1:A:458:VAL:HG12	2:B:286:THR:HG21	2.02	0.40
2:D:149:LEU:HA	2:D:150:PRO:HD3	1.96	0.40
1:A:23:GLN:HE22	1:A:60:VAL:H	1.69	0.40
4:F:804:DA:H2''	4:F:805:DG:O5'	2.22	0.40
1:C:442:VAL:HB	1:C:481:ALA:HB1	2.03	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	553/556 (100%)	539 (98%)	14 (2%)	0	100	100
1	C	554/556 (100%)	538 (97%)	16 (3%)	0	100	100
2	B	407/428 (95%)	385 (95%)	22 (5%)	0	100	100
2	D	408/428 (95%)	388 (95%)	20 (5%)	0	100	100
All	All	1922/1968 (98%)	1850 (96%)	72 (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	496/497 (100%)	495 (100%)	1 (0%)	93	98
1	C	497/497 (100%)	497 (100%)	0	100	100
2	B	373/390 (96%)	371 (100%)	2 (0%)	88	95
2	D	374/390 (96%)	368 (98%)	6 (2%)	62	84
All	All	1740/1774 (98%)	1731 (100%)	9 (0%)	88	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
2	B	277	ARG

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Mol	Chain	Res	Type
2	B	422	LEU
2	D	185	ASP
2	D	317	VAL
2	D	361	HIS
2	D	418	ASN
2	D	424	LYS
2	D	425	LEU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

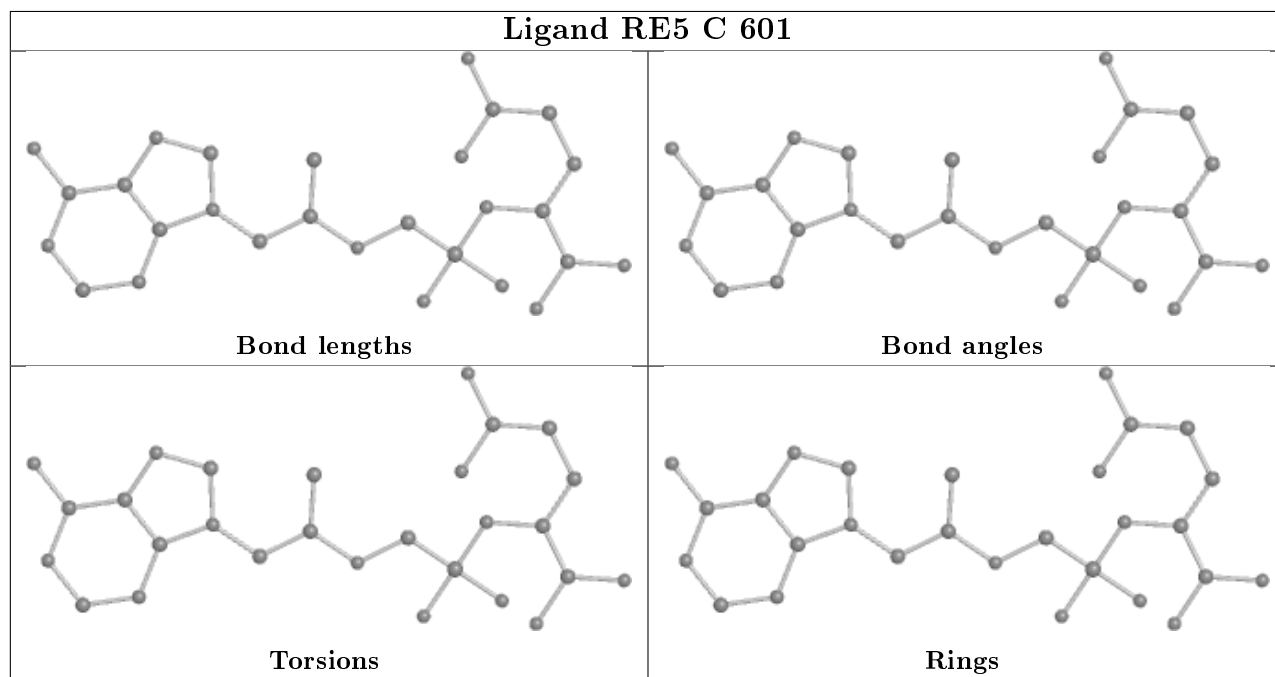
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	A	555/556 (99%)	0.94	96 (17%) 1 1	33, 103, 225, 272	0
1	C	556/556 (100%)	0.84	83 (14%) 2 1	38, 103, 221, 255	0
2	B	411/428 (96%)	0.22	12 (2%) 51 35	33, 74, 129, 160	0
2	D	412/428 (96%)	0.50	28 (6%) 17 10	44, 89, 151, 177	0
3	E	24/27 (88%)	0.67	3 (12%) 3 2	80, 142, 259, 284	0
3	T	23/27 (85%)	-0.01	2 (8%) 10 6	100, 168, 224, 289	0
4	F	18/21 (85%)	-0.20	0 100 100	71, 121, 224, 236	0
4	P	18/21 (85%)	-0.57	0 100 100	96, 132, 219, 219	0
All	All	2017/2064 (97%)	0.63	224 (11%) 5 3	33, 94, 201, 289	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	12.9
1	A	68	SER	12.2
1	A	73	LYS	12.1
1	C	63	ILE	11.3
1	C	26	LEU	10.6
1	C	133	PRO	10.1
1	A	26	LEU	9.5
3	E	702	DT	9.2
1	A	133	PRO	8.7
1	C	74	LEU	8.6
1	C	73	LYS	8.2
2	B	214	LEU	8.0
1	A	66	LYS	8.0
1	A	63	ILE	8.0
1	A	70	LYS	7.7
2	D	214	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	7.7
1	A	134	SER	7.5
1	A	142	ILE	7.5
1	A	252	TRP	7.4
3	T	703	DG	7.4
1	C	544	GLY	7.3
1	C	61	PHE	7.3
1	C	295	LEU	7.3
1	A	135	ILE	7.3
1	C	142	ILE	7.1
1	C	139	THR	6.9
1	A	62	ALA	6.7
1	A	72	ARG	6.6
1	C	32	LYS	6.6
1	A	139	THR	6.5
1	C	138	GLU	6.5
1	A	553	SER	6.5
1	C	252	TRP	6.4
1	A	65	LYS	6.4
1	A	74	LEU	6.4
1	A	138	GLU	6.3
1	A	545	ASN	6.2
1	A	289	LEU	6.2
1	C	30	LYS	6.2
1	A	34	LEU	6.2
1	A	287	LYS	6.0
1	C	132	ILE	6.0
1	A	549	ASP	5.9
1	A	286	THR	5.8
2	D	4	PRO	5.8
1	C	293	ILE	5.7
2	D	209	LEU	5.7
1	C	294	PRO	5.6
1	A	284	ARG	5.5
1	A	32	LYS	5.5
1	A	247	PRO	5.3
1	A	140	PRO	5.3
1	A	544	GLY	5.3
1	A	141	GLY	5.3
1	C	34	LEU	5.3
1	A	248	GLU	5.2
1	C	144	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	137	ASN	5.2
1	A	546	GLU	5.1
2	D	358	ARG	5.1
1	C	67	ASP	5.1
1	A	550	LYS	5.1
1	C	136	ASN	4.8
1	C	25	PRO	4.8
1	A	296	THR	4.8
1	C	49	LYS	4.7
1	C	134	SER	4.7
3	E	703	DG	4.6
1	C	246	LEU	4.5
1	A	249	LYS	4.5
1	C	62	ALA	4.5
2	D	174	GLN	4.5
3	E	704	DG	4.5
1	A	69	THR	4.3
1	A	128	THR	4.2
1	A	294	PRO	4.2
3	T	704	DG	4.2
1	A	254	VAL	4.1
1	A	246	LEU	4.1
1	C	545	ASN	4.1
1	C	135	ILE	4.1
1	A	30	LYS	4.1
1	A	64	LYS	4.1
1	A	27	THR	4.0
2	D	173	LYS	4.0
1	A	554	ALA	4.0
1	C	37	ILE	3.9
2	D	178	ILE	3.9
1	C	27	THR	3.9
1	A	282	LEU	3.9
1	C	299	ALA	3.9
1	C	281	LYS	3.9
1	A	75	VAL	3.9
1	A	137	ASN	3.8
2	B	230	MET	3.8
2	D	232	TYR	3.8
1	A	260	LEU	3.8
1	A	283	LEU	3.8
1	C	72	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	551	LEU	3.6
1	C	75	VAL	3.6
1	C	109	LEU	3.6
1	A	293	ILE	3.6
2	D	8	VAL	3.6
2	D	95	PRO	3.6
1	A	71	TRP	3.6
1	C	60	VAL	3.5
1	C	308	GLU	3.5
1	A	288	ALA	3.5
1	C	33	ALA	3.5
1	A	552	VAL	3.5
1	C	296	THR	3.5
1	C	546	GLU	3.5
2	D	168	LEU	3.5
1	C	248	GLU	3.4
1	C	69	THR	3.4
1	A	131	THR	3.4
1	A	29	GLU	3.4
2	D	202	ILE	3.4
1	A	49	LYS	3.4
1	A	136	ASN	3.4
1	A	130	PHE	3.3
1	C	140	PRO	3.3
1	C	58	THR	3.3
2	D	216	THR	3.3
1	A	28	GLU	3.3
2	B	5	ILE	3.3
1	A	60	VAL	3.3
1	A	36	GLU	3.3
2	D	361	HIS	3.2
1	C	554	ALA	3.2
1	A	251	SER	3.2
1	A	292	VAL	3.1
1	C	247	PRO	3.1
1	C	124	PHE	3.1
1	A	298	GLU	3.1
1	C	146	TYR	3.1
1	C	130	PHE	3.1
1	C	24	TRP	3.1
1	C	283	LEU	3.0
2	D	213	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	52	PRO	2.9
1	A	285	GLY	2.9
1	A	229	TRP	2.9
2	D	205	LEU	2.9
1	C	21	VAL	2.8
1	A	61	PHE	2.8
1	C	303	LEU	2.8
1	A	33	ALA	2.8
2	B	88	TRP	2.7
1	A	193	LEU	2.7
2	B	87	PHE	2.7
1	C	38	CYS	2.7
1	C	41	MET	2.7
1	C	542	ILE	2.7
1	C	29	GLU	2.6
1	A	24	TRP	2.6
2	D	88	TRP	2.6
1	A	295	LEU	2.6
1	C	36	GLU	2.6
1	A	38	CYS	2.5
1	C	249	LYS	2.5
1	A	290	THR	2.5
1	A	129	ALA	2.5
1	C	553	SER	2.5
1	C	205	LEU	2.5
2	B	213	GLY	2.5
1	C	278	GLN	2.5
1	A	299	ALA	2.4
1	C	71	TRP	2.4
1	C	65	LYS	2.4
1	A	31	ILE	2.4
2	D	171	PHE	2.4
1	C	260	LEU	2.4
1	A	271	TYR	2.4
1	A	306	ASN	2.4
1	C	551	LEU	2.4
1	A	22	LYS	2.4
1	A	303	LEU	2.4
2	B	4	PRO	2.3
2	B	85	GLN	2.3
1	C	143	ARG	2.3
1	C	292	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	41	MET	2.3
1	C	128	THR	2.3
1	C	282	LEU	2.3
2	B	91	GLN	2.3
1	A	279	LEU	2.3
2	D	242	GLN	2.2
1	A	257	ILE	2.2
1	C	279	LEU	2.2
1	A	332	GLN	2.2
2	B	301	LEU	2.2
1	C	552	VAL	2.2
1	C	15	GLY	2.2
2	D	124	PHE	2.2
1	A	302	GLU	2.2
2	D	231	GLY	2.2
1	C	547	GLN	2.2
1	A	124	PHE	2.1
1	C	311	LYS	2.1
1	A	52	PRO	2.1
2	D	10	VAL	2.1
2	D	9	PRO	2.1
1	C	22	LYS	2.1
2	B	274	ILE	2.1
1	A	144	TYR	2.1
1	A	146	TYR	2.1
2	D	5	ILE	2.1
2	D	212	TRP	2.1
1	C	214	LEU	2.1
1	C	257	ILE	2.1
2	D	154	LYS	2.1
1	C	234	LEU	2.0
2	D	146	TYR	2.0
2	B	93	GLY	2.0
1	A	245	VAL	2.0
2	D	94	ILE	2.0
1	A	547	GLN	2.0
1	C	277	ARG	2.0
1	A	297	GLU	2.0
1	C	291	GLU	2.0
1	A	48	SER	2.0

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
4	MRG	P	817	22/27	0.86	0.10	134,161,168,173	0
4	MRG	F	817	22/27	0.91	0.15	107,134,149,158	0
4	DDG	F	822	21/22	0.94	0.18	81,104,116,131	0
4	DDG	P	822	21/22	0.96	0.11	82,99,112,117	0

6.3 Carbohydrates [i](#)

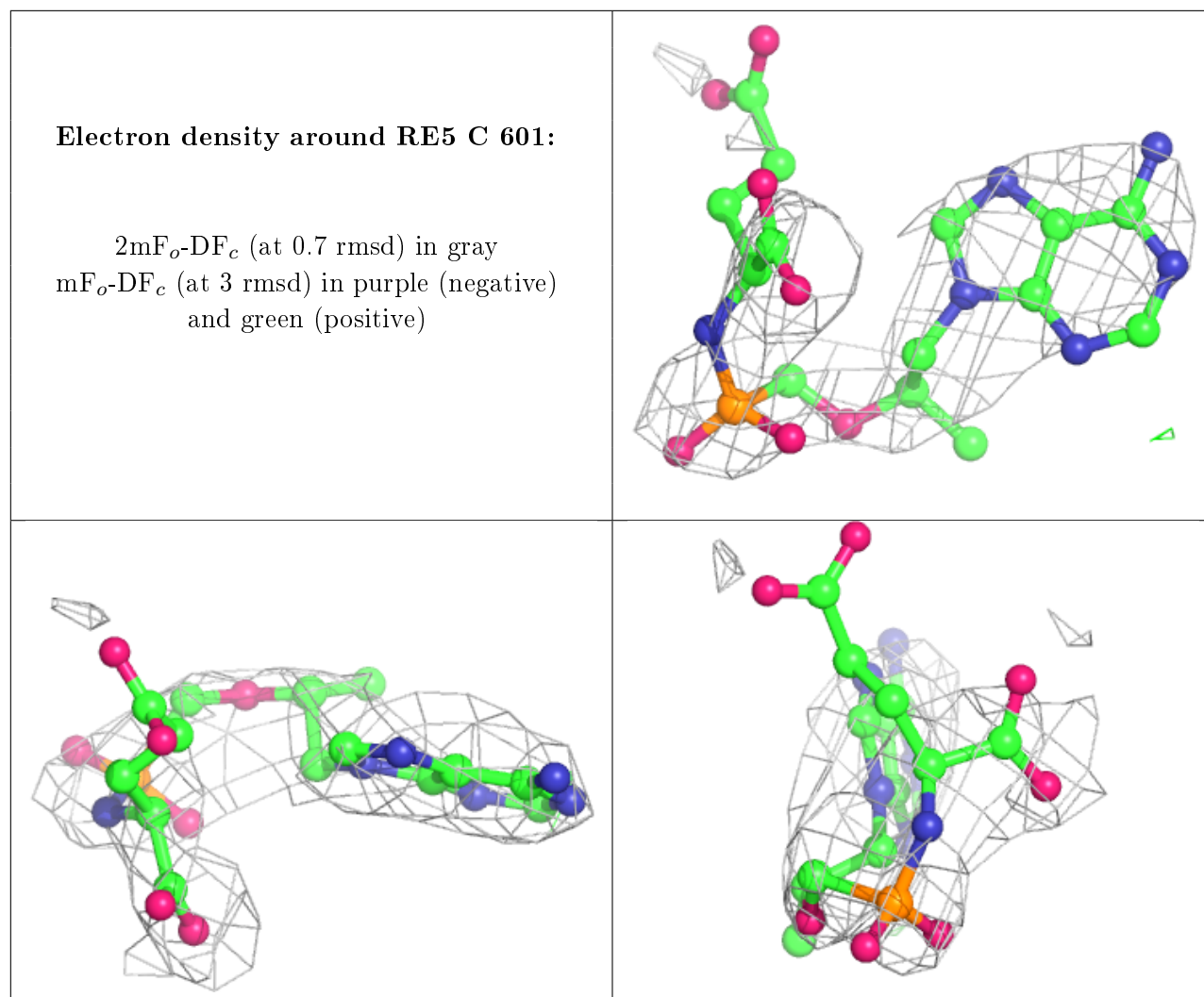
There are no monosaccharides in this entry.

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, 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
5	RE5	C	601	28/28	0.80	0.27	137,159,188,192	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.