



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:05 PM UTC

PDB ID : 7AIJ / pdb_00007aij
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEX WITH DNA AND L-METHIONINE 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 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:

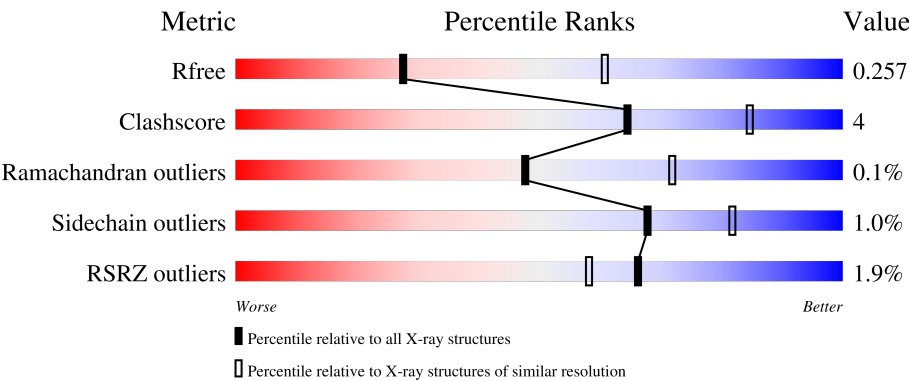
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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.



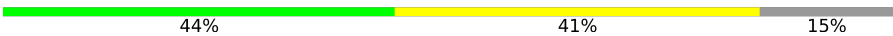
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	3% 90% 9% .
1	C	556	3% 88% 12%
2	B	428	% 87% 8% . .
2	D	428	% 85% 11% .

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Mol	Chain	Length	Quality of chain
3	E	27	 48% 37% 15%
3	T	27	 44% 41% 15%
4	F	21	 62% 29% 5% 5%
4	P	21	 76% 14% 5% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17687 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
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
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

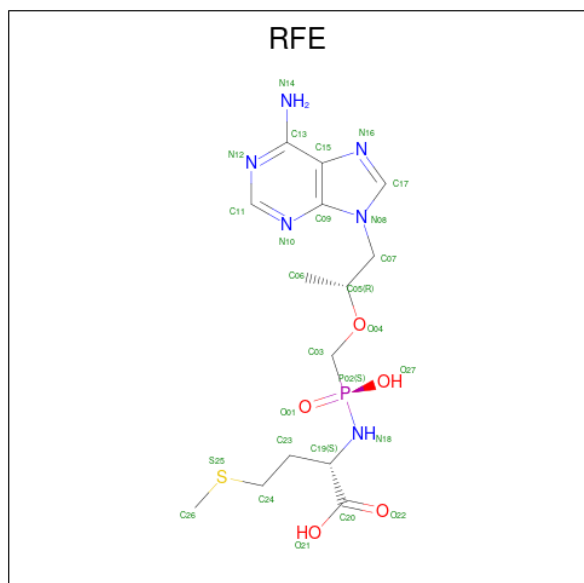
- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3').

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	23	Total	C	N	O	P	0	0	0
			477	223	95	136	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-Methionine Tenofovir (CCD ID: RFE) (formula: C₁₄H₂₃N₆O₅PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			27	14	6	5	1	1		

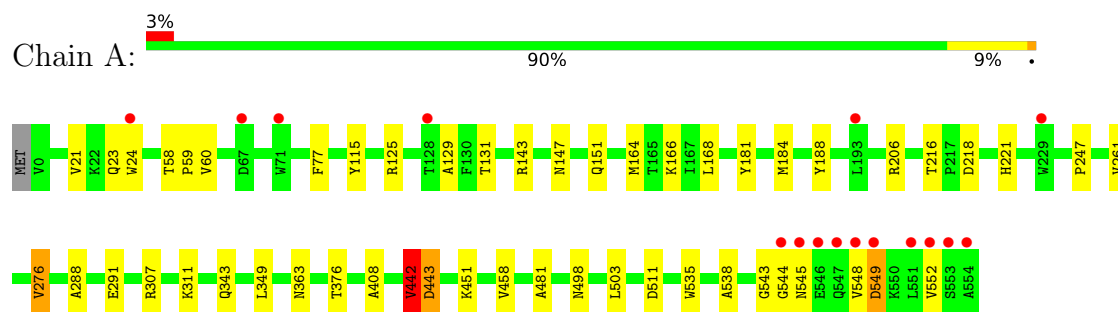
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	17	Total 17	O 17	0	0
6	B	17	Total 17	O 17	0	0
6	C	14	Total 14	O 14	0	0
6	D	10	Total 10	O 10	0	0
6	T	4	Total 4	O 4	0	0
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

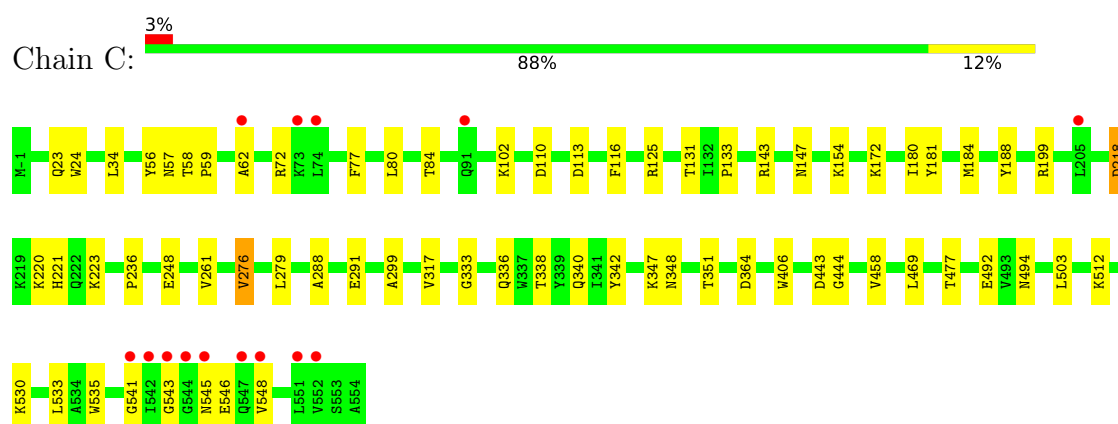
3 Residue-property plots [i](#)

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.

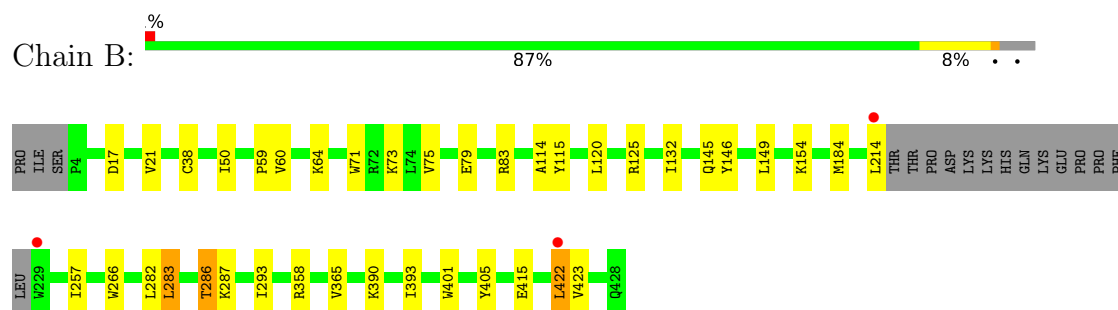
• Molecule 1: Gag-Pol polyprotein



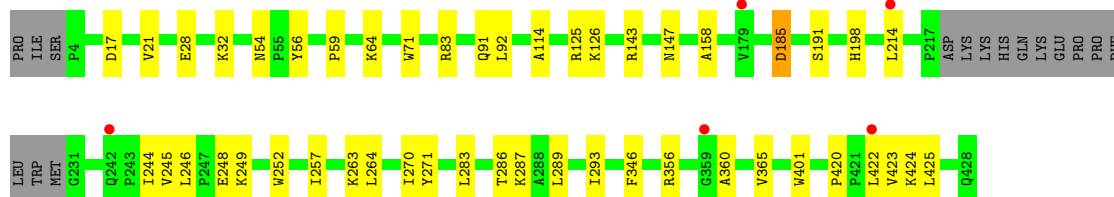
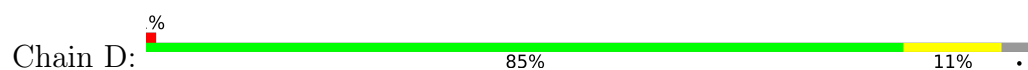
• Molecule 1: Gag-Pol polyprotein



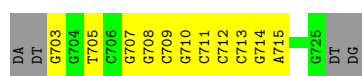
• Molecule 2: Gag-Pol polyprotein



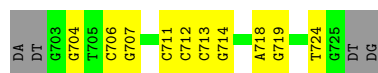
• Molecule 2: Gag-Pol polyprotein



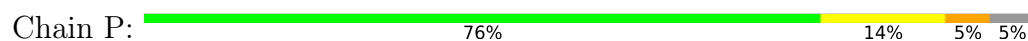
- Molecule 3: DNA (5'-D(P*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*A P*GP*GP*GP*AP*CP*TP*G)-3')



- Molecule 3: DNA (5'-D(P*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*A P*GP*GP*GP*AP*CP*TP*G)-3')



- 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')



- 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')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.62Å 132.93Å 139.98Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	69.22 – 2.95 69.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (69.22-2.95) 99.5 (69.22-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.226 , 0.263 0.226 , 0.257	Depositor DCC
R_{free} test set	1971 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17687	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: RFE, DDG, MRG

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	0.08	0/4631	0.24	0/6293
1	C	0.08	0/4639	0.23	0/6303
2	B	0.08	0/3499	0.24	0/4752
2	D	0.08	0/3497	0.23	0/4751
3	E	0.16	0/536	0.30	0/826
3	T	0.16	0/536	0.30	0/826
4	F	0.22	0/400	0.42	0/612
4	P	0.19	0/400	0.36	0/612
All	All	0.09	0/18138	0.25	0/24975

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	34	0
1	C	4521	0	4587	38	0
2	B	3401	0	3431	25	0
2	D	3400	0	3433	26	0
3	E	477	0	256	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	477	0	256	7	0
4	F	403	0	224	6	0
4	P	403	0	224	3	0
5	C	27	0	0	1	0
6	A	17	0	0	1	0
6	B	17	0	0	0	0
6	C	14	0	0	0	0
6	D	10	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	T	4	0	0	0	0
All	All	17687	0	16989	131	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 (131) 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)
1:C:543:GLY:N	2:D:283:LEU:O	2.26	0.67
1:C:56:TYR:O	1:C:143:ARG:NH2	2.29	0.65
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.79	0.65
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.79	0.64
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.79	0.63
1:C:545:ASN:HA	1:C:548:VAL:HG12	1.80	0.63
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.80	0.62
1:C:172:LYS:HE2	1:C:180:ILE:HB	1.82	0.61
1:C:125:ARG:HE	1:C:147:ASN:HA	1.65	0.61
1:A:544:GLY:HA3	2:B:286:THR:HG23	1.82	0.61
1:C:184:MET:HG2	4:F:822:DDG:H2'	1.82	0.61
1:A:115:TYR:HD2	1:A:151:GLN:HG2	1.67	0.60
2:D:56:TYR:HE2	2:D:126:LYS:HE2	1.67	0.60
1:C:110:ASP:HB2	1:C:220:LYS:HD3	1.82	0.59
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.83	0.59
1:C:102:LYS:NZ	1:C:236:PRO:O	2.32	0.59
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.70	0.57
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.87	0.56
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.88	0.56
2:D:125:ARG:NH1	2:D:147:ASN:O	2.38	0.56
1:A:206:ARG:NH2	1:A:216:THR:O	2.39	0.56
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.31	0.55
1:C:469:LEU:HD12	1:C:477:THR:HG22	1.87	0.55
2:D:356:ARG:HD2	2:D:360:ALA:HB1	1.88	0.55
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.40	0.55
1:C:72:ARG:NH2	5:C:601:RFE:O21	2.30	0.55
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.89	0.54
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.89	0.54
2:D:422:LEU:HD23	2:D:422:LEU:H	1.73	0.54
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.54
1:A:451:LYS:NZ	4:P:808:DC:OP1	2.42	0.52
1:C:364:ASP:OD1	1:C:512:LYS:NZ	2.32	0.52
1:A:545:ASN:OD1	6:A:601:HOH:O	2.19	0.52
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.91	0.52
2:D:191:SER:OG	2:D:198:HIS:ND1	2.32	0.52
3:E:724:DT:H3	4:F:804:DA:H61	1.58	0.51
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.92	0.51
2:B:358:ARG:NH2	2:B:405:TYR:O	2.34	0.51
1:C:458:VAL:HG12	2:D:286:THR:HG21	1.92	0.51
2:B:60:VAL:HG22	2:B:75:VAL:HG22	1.93	0.51
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.46	0.50
1:C:443:ASP:OD1	1:C:444:GLY:N	2.44	0.50
3:E:718:DA:H1'	3:E:719:DG:C8	2.46	0.50
1:A:23:GLN:HE22	1:A:60:VAL:H	1.60	0.49
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.94	0.49
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.95	0.49
1:C:113:ASP:HB3	1:C:116:PHE:HB2	1.95	0.48
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.95	0.48
2:D:245:VAL:O	2:D:263:LYS:NZ	2.43	0.48
1:A:548:VAL:O	1:A:552:VAL:HG22	2.14	0.48
2:B:266:TRP:CE2	2:B:422:LEU:HD13	2.49	0.47
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.95	0.47
2:D:244:ILE:HD12	2:D:271:TYR:HE1	1.79	0.47
2:D:114:ALA:HB2	2:D:214:LEU:HD13	1.97	0.47
3:T:709:DC:H2'	3:T:710:DG:C8	2.48	0.47
1:A:58:THR:HG21	1:A:77:PHE:CE1	2.51	0.46
2:D:28:GLU:HG2	2:D:32:LYS:HE2	1.96	0.46
2:D:92:LEU:HB2	2:D:158:ALA:HB1	1.97	0.46
3:T:709:DC:H2'	3:T:710:DG:H8	1.81	0.46
1:A:543:GLY:H	2:B:283:LEU:C	2.22	0.46
1:C:342:TYR:HB3	1:C:348:ASN:HA	1.98	0.46
1:A:443:ASP:HB2	1:A:498:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:711:DC:H2'	3:E:712:DC:C6	2.51	0.46
1:A:543:GLY:N	2:B:283:LEU:O	2.39	0.46
1:A:24:TRP:HD1	1:A:59:PRO:HB3	1.81	0.45
1:C:199:ARG:HH12	1:C:223:LYS:HB3	1.82	0.45
2:D:249:LYS:HB2	2:D:252:TRP:CE2	2.51	0.45
1:C:317:VAL:HG11	1:C:347:LYS:HB3	1.99	0.45
1:C:80:LEU:O	1:C:84:THR:OG1	2.30	0.45
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.97	0.45
1:C:541:GLY:HA2	1:C:546:GLU:HB2	1.98	0.45
3:T:711:DC:H2'	3:T:712:DC:C6	2.51	0.45
3:E:704:DG:OP2	3:E:704:DG:N2	2.50	0.45
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.82	0.44
2:D:270:ILE:HG12	2:D:346:PHE:HB3	1.99	0.44
1:C:57:ASN:HD21	1:C:131:THR:HG22	1.81	0.44
1:C:84:THR:HB	1:C:154:LYS:HE2	2.00	0.44
2:D:17:ASP:O	2:D:83:ARG:HD3	2.16	0.44
1:A:184:MET:HG2	4:P:822:DDG:H2'	1.99	0.44
3:T:703:DG:H21	3:T:705:DT:H73	1.82	0.44
1:C:279:LEU:HD23	1:C:299:ALA:HB1	2.00	0.44
1:C:503:LEU:HD12	1:C:533:LEU:HD13	2.00	0.44
2:D:185:ASP:OD1	2:D:185:ASP:N	2.48	0.43
1:A:164:MET:HE3	1:A:168:LEU:HD11	2.01	0.43
2:B:154:LYS:HG2	2:B:184:MET:SD	2.58	0.43
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.99	0.43
1:A:545:ASN:O	1:A:549:ASP:HB2	2.19	0.43
1:C:218:ASP:HA	1:C:221:HIS:HB2	2.01	0.43
4:F:818:DC:H2'	4:F:819:DG:C8	2.54	0.43
1:A:58:THR:HG22	1:A:129:ALA:O	2.18	0.43
2:D:287:LYS:HD3	2:D:293:ILE:HD11	2.00	0.43
3:T:714:DG:H2''	3:T:715:DA:C8	2.54	0.43
4:P:818:DC:H2'	4:P:819:DG:C8	2.53	0.43
4:F:814:DC:H2''	4:F:815:DG:C8	2.55	0.42
2:B:422:LEU:H	2:B:422:LEU:HG	1.49	0.42
2:D:257:ILE:HB	2:D:283:LEU:HD21	2.02	0.42
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.54	0.42
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.00	0.42
3:E:706:DC:H2'	3:E:707:DG:C8	2.54	0.42
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.54	0.42
3:T:707:DG:H2'	3:T:708:DG:C8	2.55	0.42
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.90	0.42
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:O	1:A:307:ARG:NH2	2.53	0.41
2:B:17:ASP:O	2:B:83:ARG:HD3	2.19	0.41
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.41
2:D:21:VAL:HB	2:D:59:PRO:HD3	2.02	0.41
1:C:23:GLN:HG2	1:C:133:PRO:HD3	2.03	0.41
1:A:498:ASN:HD22	1:A:538:ALA:HB2	1.84	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.03	0.41
1:C:24:TRP:HD1	1:C:59:PRO:HB3	1.84	0.41
2:D:91:GLN:HG2	2:D:92:LEU:HG	2.02	0.41
4:F:804:DA:H2''	4:F:805:DG:O5'	2.21	0.41
4:F:818:DC:H2'	4:F:819:DG:H8	1.84	0.41
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.41
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.03	0.41
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.01	0.41
1:C:199:ARG:NH1	1:C:223:LYS:HB3	2.36	0.41
1:C:58:THR:HG21	1:C:77:PHE:CD1	2.56	0.41
1:A:307:ARG:O	1:A:311:LYS:HG3	2.21	0.40
3:T:713:DC:H2'	3:T:714:DG:C8	2.56	0.40
1:A:408:ALA:O	2:B:393:ILE:HG13	2.22	0.40
1:A:218:ASP:HA	1:A:221:HIS:HB2	2.03	0.40
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.04	0.40
2:B:50:ILE:HD13	2:B:145:GLN:HB3	2.03	0.40
1:C:34:LEU:HD21	1:C:62:ALA:HB2	2.03	0.40
1:C:333:GLY:H	1:C:336:GLN:HB2	1.86	0.40
3:E:713:DC:H2'	3:E:714:DG:C8	2.57	0.40
1:C:340:GLN:HG3	1:C:351:THR:HG22	2.03	0.40
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.22	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%)	534 (97%)	18 (3%)	1 (0%)	43	66
1	C	554/556 (100%)	536 (97%)	18 (3%)	0	100	100
2	B	407/428 (95%)	390 (96%)	17 (4%)	0	100	100
2	D	408/428 (95%)	388 (95%)	20 (5%)	0	100	100
All	All	1922/1968 (98%)	1848 (96%)	73 (4%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/497 (100%)	492 (99%)	4 (1%)	73	85
1	C	497/497 (100%)	493 (99%)	4 (1%)	73	85
2	B	373/390 (96%)	368 (99%)	5 (1%)	61	78
2	D	374/390 (96%)	369 (99%)	5 (1%)	61	78
All	All	1740/1774 (98%)	1722 (99%)	18 (1%)	68	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	442	VAL
1	A	443	ASP
1	A	549	ASP
2	B	282	LEU
2	B	283	LEU
2	B	286	THR
2	B	422	LEU
2	B	423	VAL
1	C	218	ASP

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Mol	Chain	Res	Type
1	C	248	GLU
1	C	276	VAL
1	C	338	THR
2	D	185	ASP
2	D	248	GLU
2	D	423	VAL
2	D	424	LYS
2	D	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	315	HIS
1	A	407	GLN
2	B	265	ASN
2	B	269	GLN
2	B	373	GLN
2	B	428	GLN
1	C	147	ASN
1	C	255	ASN
1	C	336	GLN
1	C	407	GLN
1	C	520	GLN
1	C	524	GLN
1	C	547	GLN
2	D	235	HIS
2	D	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
4	MRG	F	817	3,4	21,24,29	0.41	0	30,35,42	0.36	0
4	DDG	F	822	3,4	20,23,24	0.81	0	27,33,36	2.13	10 (37%)
4	MRG	P	817	3,4	21,24,29	0.39	0	30,35,42	0.36	0
4	DDG	P	822	3,4	20,23,24	0.82	0	27,33,36	2.10	8 (29%)

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
4	MRG	F	817	3,4	-	0/7/21/27	0/3/3/3
4	DDG	F	822	3,4	-	1/7/18/19	0/3/3/3
4	MRG	P	817	3,4	-	0/7/21/27	0/3/3/3
4	DDG	P	822	3,4	-	0/7/18/19	0/3/3/3

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	822	DDG	C5-C4-N3	-5.47	119.68	128.39
4	P	822	DDG	C5-C4-N3	-5.41	119.79	128.39
4	F	822	DDG	C2-N3-C4	5.09	121.06	112.30
4	P	822	DDG	C2-N3-C4	5.06	121.02	112.30
4	F	822	DDG	N9-C4-N3	4.09	134.12	125.95
4	P	822	DDG	N9-C4-N3	4.03	134.01	125.95
4	F	822	DDG	C8-N7-C5	2.82	109.29	104.26
4	P	822	DDG	C8-N7-C5	2.81	109.26	104.26
4	F	822	DDG	C2-N1-C6	-2.67	120.26	125.11
4	P	822	DDG	C2-N1-C6	-2.66	120.28	125.11
4	F	822	DDG	C4-C5-N7	-2.20	107.18	110.67
4	P	822	DDG	C4-C5-N7	-2.19	107.21	110.67
4	P	822	DDG	O6-C6-C5	-2.17	120.80	126.53
4	P	822	DDG	C6-C5-N7	2.17	134.24	130.29
4	F	822	DDG	C6-C5-N7	2.17	134.24	130.29
4	F	822	DDG	O6-C6-C5	-2.15	120.86	126.53
4	F	822	DDG	C5-C6-N1	2.01	118.37	113.25
4	F	822	DDG	C4'-O4'-C1'	-2.01	107.91	109.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	822	DDG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	822	DDG	1	0
4	P	822	DDG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	RFE	C	601	-	25,28,28	2.03	11 (44%)	30,39,39	2.17	8 (26%)

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	RFE	C	601	-	-	8/20/23/23	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	601	RFE	C07-N08	4.34	1.52	1.46
5	C	601	RFE	C17-N08	3.67	1.42	1.36
5	C	601	RFE	C09-N08	3.18	1.41	1.37
5	C	601	RFE	C15-C09	2.98	1.44	1.39
5	C	601	RFE	C07-C05	2.78	1.61	1.51
5	C	601	RFE	P02-O27	-2.53	1.50	1.56
5	C	601	RFE	C09-N10	2.34	1.38	1.34
5	C	601	RFE	C23-C19	2.30	1.58	1.53
5	C	601	RFE	C19-C20	2.23	1.58	1.52
5	C	601	RFE	C11-N12	2.11	1.37	1.33
5	C	601	RFE	C17-N16	2.10	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	RFE	O27-P02-O01	5.44	126.47	112.36
5	C	601	RFE	C07-N08-C09	5.11	132.33	126.41
5	C	601	RFE	C05-C07-N08	4.69	120.09	112.68
5	C	601	RFE	N10-C09-N08	3.57	131.29	126.87
5	C	601	RFE	C15-C09-N10	-3.28	122.20	126.72
5	C	601	RFE	C23-C19-C20	-2.43	104.58	110.35
5	C	601	RFE	C07-N08-C17	-2.42	122.75	126.63
5	C	601	RFE	C23-C19-N18	2.36	115.29	111.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

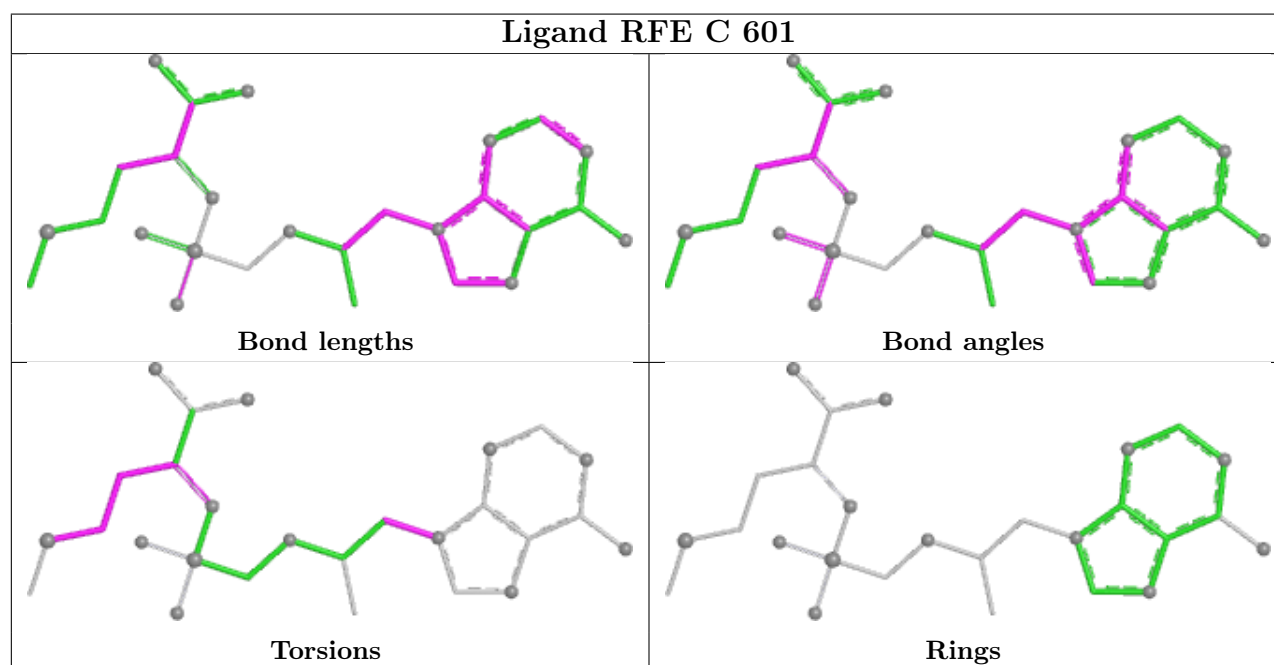
Mol	Chain	Res	Type	Atoms
5	C	601	RFE	C05-C07-N08-C17
5	C	601	RFE	C20-C19-C23-C24
5	C	601	RFE	N18-C19-C23-C24
5	C	601	RFE	C19-C23-C24-S25
5	C	601	RFE	C23-C24-S25-C26
5	C	601	RFE	C05-C07-N08-C09
5	C	601	RFE	C20-C19-N18-P02
5	C	601	RFE	C23-C19-N18-P02

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	RFE	1	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 ⓘ

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, 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%)	0.09	16 (2%) 53 46	41, 116, 214, 272	0
1	C	556/556 (100%)	0.05	14 (2%) 58 50	43, 119, 211, 243	0
2	B	411/428 (96%)	-0.17	3 (0%) 84 80	40, 88, 140, 169	0
2	D	412/428 (96%)	-0.11	5 (1%) 76 71	52, 100, 160, 185	0
3	E	23/27 (85%)	-0.30	0 100 100	96, 146, 209, 249	0
3	T	23/27 (85%)	-0.27	0 100 100	108, 156, 205, 267	0
4	F	18/21 (85%)	-0.63	0 100 100	83, 129, 207, 209	0
4	P	18/21 (85%)	-0.68	0 100 100	97, 141, 198, 200	0
All	All	2016/2064 (97%)	-0.04	38 (1%) 66 58	40, 106, 191, 272	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	544	GLY	6.7
1	A	544	GLY	5.3
1	A	545	ASN	4.9
1	C	545	ASN	4.7
1	C	551	LEU	4.7
1	A	67	ASP	4.0
1	A	551	LEU	3.8
1	C	542	ILE	3.7
1	C	552	VAL	3.7
1	A	549	ASP	3.5
1	A	552	VAL	3.4
1	C	543	GLY	3.4
1	C	548	VAL	3.3
1	A	548	VAL	3.1
2	D	359	GLY	3.0
1	A	71	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	541	GLY	2.6
1	C	547	GLN	2.5
2	B	229	TRP	2.5
1	A	554	ALA	2.5
2	D	214	LEU	2.5
1	C	205	LEU	2.4
1	A	24	TRP	2.4
1	A	193	LEU	2.4
2	B	422	LEU	2.4
1	C	74	LEU	2.3
1	C	91	GLN	2.3
1	A	546	GLU	2.3
1	A	128	THR	2.2
1	A	229	TRP	2.2
1	A	553	SER	2.1
2	D	242	GLN	2.1
2	D	422	LEU	2.1
2	D	179	VAL	2.1
1	C	62	ALA	2.1
1	A	547	GLN	2.0
2	B	214	LEU	2.0
1	C	73	LYS	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	0.72	0.08	138,158,172,174	0
4	MRG	F	817	22/27	0.81	0.07	124,140,155,170	0
4	DDG	P	822	21/22	0.86	0.09	104,118,127,129	0
4	DDG	F	822	21/22	0.90	0.10	103,119,126,130	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

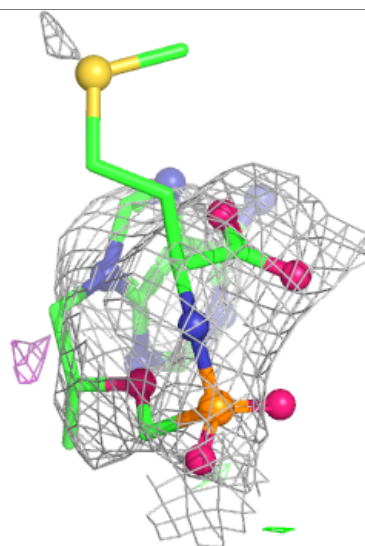
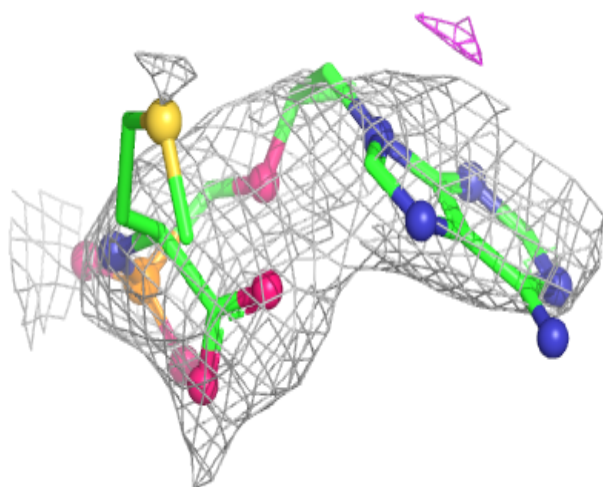
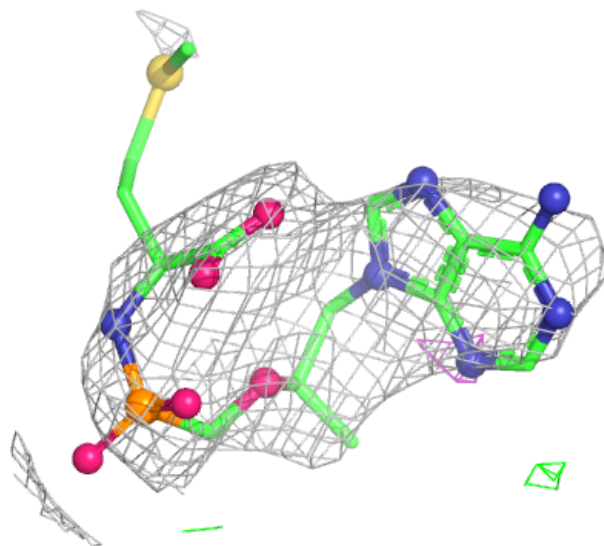
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	RFE	C	601	27/27	0.72	0.13	143,168,190,201	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.

Electron density around RFE C 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.