



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:28 PM UTC

PDB ID : 6UJZ / pdb_00006ujz
Title : HIV-1 wild-type reverse transcriptase-DNA complex with (+)-FTC-TP
Authors : Lansdon, E.B.
Deposited on : 2019-10-03
Resolution : 2.56 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

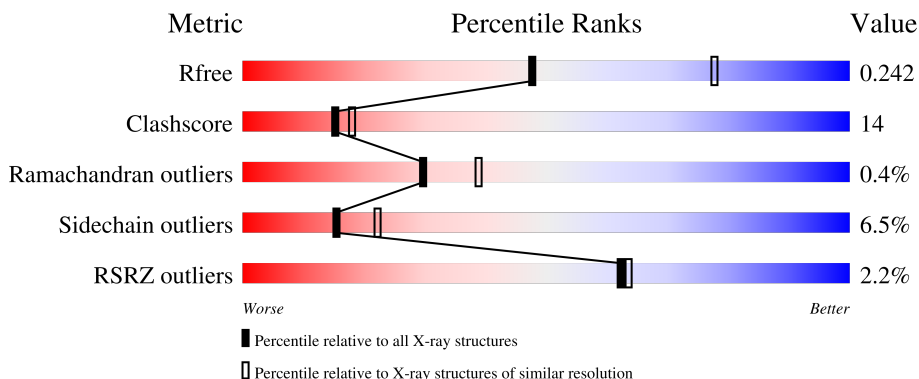
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	572	69% 24% • •
2	B	440	61% 27% • 9%
3	P	21	43% 43% 14%
4	T	27	48% 41% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8743 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 p66 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4500	2910	752	830	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P04585
A	-10	GLY	-	expression tag	UNP P04585
A	-9	SER	-	expression tag	UNP P04585
A	-8	SER	-	expression tag	UNP P04585
A	-7	HIS	-	expression tag	UNP P04585
A	-6	HIS	-	expression tag	UNP P04585
A	-5	HIS	-	expression tag	UNP P04585
A	-4	HIS	-	expression tag	UNP P04585
A	-3	HIS	-	expression tag	UNP P04585
A	-2	HIS	-	expression tag	UNP P04585
A	-1	SER	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called p51 Reverse transcriptase/RNaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	0	0
			3295	2139	550	600	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585

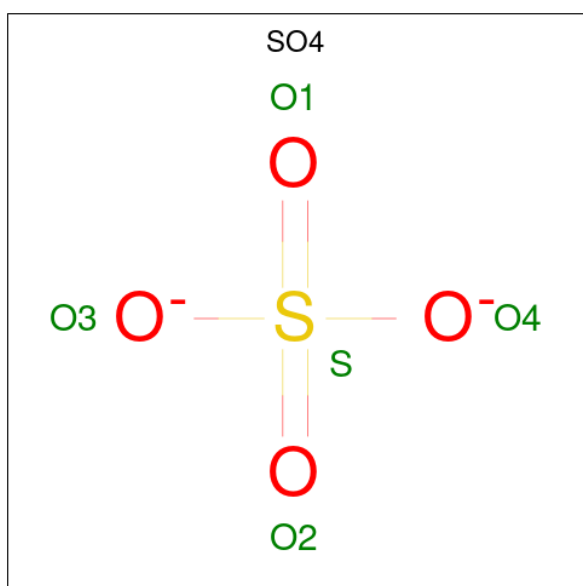
- Molecule 3 is a DNA chain called primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	P	0	0	0
			360	172	62	109	17			

- Molecule 4 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	24	Total	C	N	O	P	0	0	0
			502	234	102	142	24			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



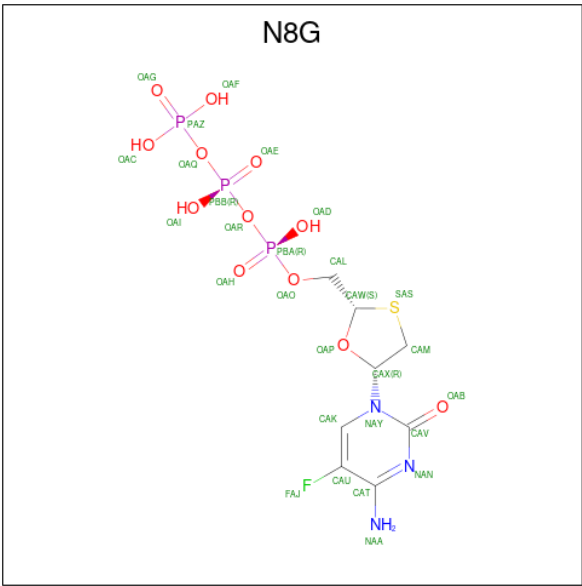
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is [[(2 {S},5 {R})-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (CCD ID:

N8G) (formula: C₈H₁₃FN₃O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	P	S	0	0
			28	8	1	3	12	3	1		

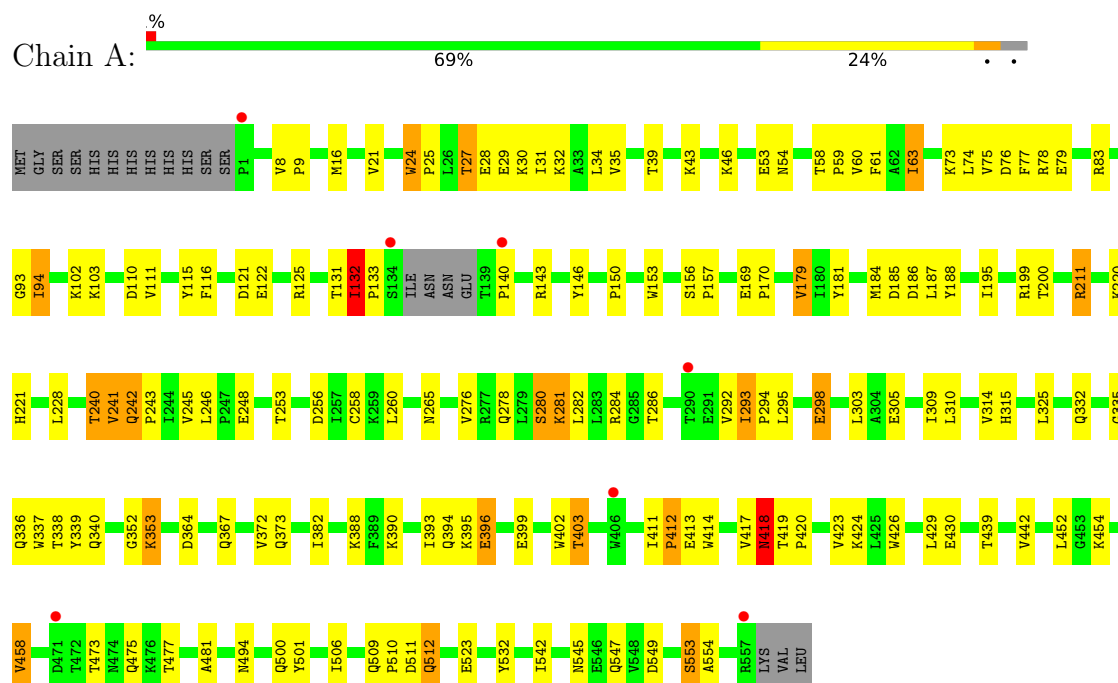
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total	O	0	0
			23	23		
8	B	19	Total	O	0	0
			19	19		
8	P	3	Total	O	0	0
			3	3		
8	T	2	Total	O	0	0
			2	2		

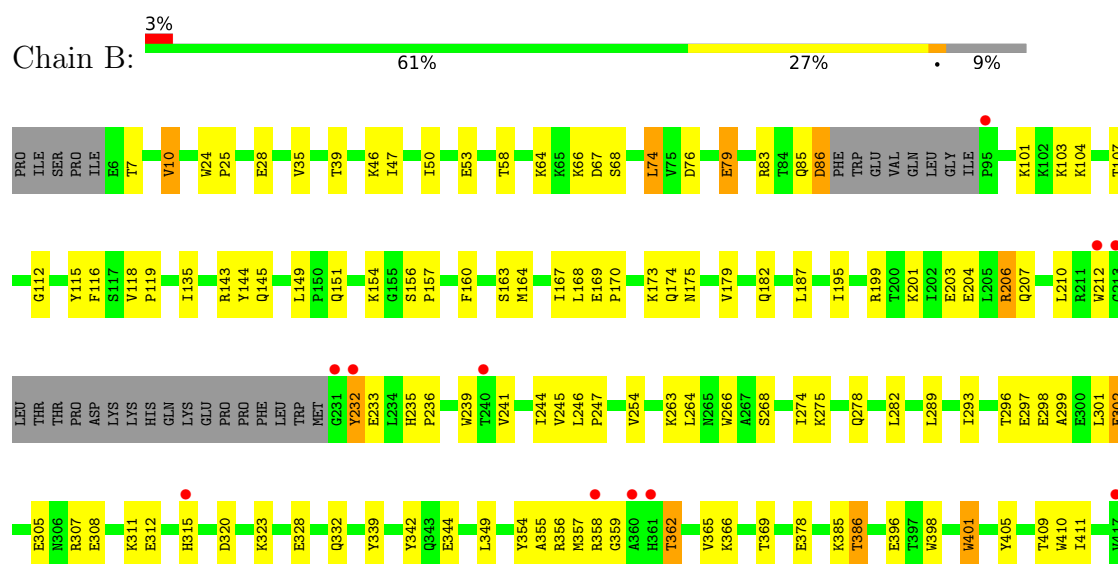
3 Residue-property plots

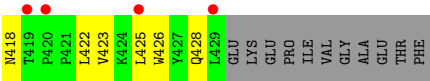
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: p66 Reverse transcriptase/RNaseH

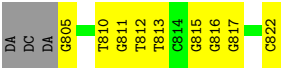


• Molecule 2: p51 Reverse transcriptase/RNaseH

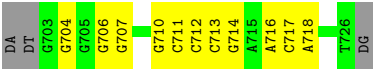




● Molecule 3: primer DNA



● Molecule 4: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	168.28Å 168.83Å 102.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.34 – 2.56 47.34 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.34-2.56) 90.0 (47.34-2.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692, PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.236 0.192 , 0.242	Depositor DCC
R_{free} test set	1999 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8743	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, MG, N8G, SO4

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	0.61	0/4616	0.93	9/6269 (0.1%)
2	B	0.56	0/3386	0.87	5/4596 (0.1%)
3	P	0.40	0/381	0.55	0/586
4	T	0.46	0/565	0.54	0/872
All	All	0.58	0/8948	0.87	14/12323 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ILE	CA-C-N	11.78	131.91	119.78
1	A	132	ILE	C-N-CA	11.78	131.91	119.78
2	B	386	THR	CA-C-N	-6.69	113.90	120.52
2	B	386	THR	C-N-CA	-6.69	113.90	120.52
1	A	382	ILE	N-CA-C	5.83	116.01	110.53
1	A	132	ILE	O-C-N	5.74	125.62	121.55
2	B	344	GLU	CA-C-N	5.73	127.00	119.84
2	B	344	GLU	C-N-CA	5.73	127.00	119.84
1	A	94	ILE	CA-C-N	-5.68	114.11	119.85
1	A	94	ILE	C-N-CA	-5.68	114.11	119.85
2	B	401	TRP	N-CA-C	5.15	121.28	114.12
1	A	458	VAL	N-CA-C	-5.12	101.26	108.27
1	A	242	GLN	CA-C-N	5.05	126.15	119.84
1	A	242	GLN	C-N-CA	5.05	126.15	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4500	0	4557	116	0
2	B	3295	0	3326	103	0
3	P	360	0	203	8	0
4	T	502	0	267	15	0
5	A	10	0	0	0	0
6	A	1	0	0	0	0
7	A	28	0	0	0	0
8	A	23	0	0	0	0
8	B	19	0	0	3	0
8	P	3	0	0	1	0
8	T	2	0	0	0	0
All	All	8743	0	8353	232	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 14.

All (232) 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:232:TYR:HB3	2:B:233:GLU:HG3	1.41	1.02
1:A:402:TRP:CE3	1:A:403:THR:HG22	2.03	0.93
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.55	0.88
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.57	0.86
4:T:717:DC:H2''	4:T:718:DA:H5'	1.59	0.84
1:A:286:THR:HG21	1:A:293:ILE:CD1	2.07	0.84
4:T:704:DG:H5''	4:T:704:DG:N3	1.93	0.84
1:A:399:GLU:O	1:A:403:THR:HG23	1.80	0.82
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.15	0.81
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.61	0.81
2:B:35:VAL:O	2:B:39:THR:HG23	1.81	0.81
2:B:365:VAL:O	2:B:369:THR:HG23	1.80	0.80
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.47	0.79
2:B:167:ILE:HG23	2:B:212:TRP:HE3	1.47	0.79
2:B:254:VAL:HG22	2:B:293:ILE:HD11	1.65	0.77
2:B:232:TYR:CB	2:B:233:GLU:HG3	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.68	0.76
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.22	0.74
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.68	0.74
2:B:247:PRO:O	2:B:307:ARG:NH2	2.20	0.74
2:B:46:LYS:HE3	2:B:116:PHE:CD2	2.22	0.72
1:A:402:TRP:CZ3	1:A:403:THR:HG22	2.23	0.72
1:A:63:ILE:HD13	1:A:74:LEU:HD11	1.71	0.72
2:B:79:GLU:HG3	2:B:83:ARG:NH1	2.03	0.72
4:T:716:DA:H2'	4:T:717:DC:C6	2.26	0.71
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.73	0.71
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.17	0.70
2:B:278:GLN:HG3	2:B:298:GLU:HB3	1.73	0.70
2:B:357:MET:CE	2:B:359:GLY:HA3	2.22	0.69
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.74	0.68
2:B:254:VAL:HG22	2:B:293:ILE:CD1	2.22	0.68
1:A:27:THR:HG22	1:A:29:GLU:H	1.56	0.68
1:A:131:THR:HG22	1:A:143:ARG:CG	2.24	0.68
3:P:816:DG:H2'	3:P:817:DG:C8	2.30	0.67
1:A:110:ASP:HB3	1:A:220:LYS:HD2	1.76	0.67
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.76	0.66
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.30	0.65
1:A:35:VAL:O	1:A:39:THR:HG23	1.96	0.65
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.78	0.65
1:A:27:THR:HG22	1:A:29:GLU:N	2.12	0.64
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.79	0.64
1:A:258:CYS:SG	8:P:901:HOH:O	2.55	0.63
1:A:281:LYS:NZ	1:A:284:ARG:HD3	2.14	0.63
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.81	0.63
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.30	0.62
3:P:816:DG:H2'	3:P:817:DG:H8	1.64	0.62
2:B:297:GLU:O	2:B:301:LEU:HG	2.00	0.62
2:B:107:THR:HG23	2:B:232:TYR:HD1	1.64	0.61
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.36	0.61
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.31	0.61
3:P:812:DT:H2''	3:P:813:DT:H5'	1.83	0.61
1:A:30:LYS:O	1:A:34:LEU:HG	2.01	0.61
1:A:211:ARG:HD2	1:A:211:ARG:C	2.25	0.60
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.36	0.60
4:T:713:DC:H2'	4:T:714:DG:C8	2.37	0.60
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.84	0.59
1:A:511:ASP:OD1	1:A:512:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.38	0.59
1:A:332:GLN:HB2	1:A:336:GLN:O	2.02	0.59
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.85	0.58
2:B:167:ILE:O	2:B:212:TRP:HZ3	1.85	0.58
1:A:46:LYS:HE2	1:A:116:PHE:O	2.04	0.58
1:A:424:LYS:HE3	1:A:426:TRP:CD2	2.39	0.58
1:A:73:LYS:HE3	1:A:146:TYR:OH	2.03	0.58
4:T:712:DC:H2'	4:T:713:DC:C6	2.39	0.58
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.33	0.57
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.39	0.57
1:A:211:ARG:C	1:A:211:ARG:CD	2.77	0.57
2:B:85:GLN:NE2	8:B:501:HOH:O	2.38	0.57
1:A:28:GLU:HA	1:A:31:ILE:HD12	1.87	0.56
1:A:131:THR:HG22	1:A:143:ARG:CD	2.35	0.56
2:B:323:LYS:O	2:B:385:LYS:HE2	2.05	0.56
2:B:195:ILE:O	2:B:199:ARG:HG3	2.06	0.56
4:T:716:DA:H2'	4:T:717:DC:H6	1.68	0.56
1:A:276:VAL:HG22	1:A:353:LYS:HE3	1.88	0.56
2:B:195:ILE:CG1	2:B:199:ARG:HH11	2.19	0.56
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.41	0.56
1:A:454:LYS:NZ	1:A:554:ALA:O	2.30	0.55
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.72	0.55
4:T:717:DC:H2'	4:T:718:DA:C8	2.40	0.55
1:A:110:ASP:CB	1:A:220:LYS:HD2	2.37	0.55
4:T:711:DC:H2'	4:T:712:DC:C6	2.42	0.55
2:B:203:GLU:O	2:B:207:GLN:HG3	2.07	0.55
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.89	0.54
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.89	0.54
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.07	0.54
1:A:103:LYS:HE3	1:A:179:VAL:CG1	2.38	0.54
2:B:320:ASP:OD2	2:B:323:LYS:HG3	2.08	0.54
2:B:107:THR:CG2	2:B:232:TYR:HD1	2.21	0.54
1:A:278:GLN:O	1:A:282:LEU:HD13	2.08	0.53
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.09	0.53
2:B:103:LYS:NZ	2:B:179:VAL:HG23	2.24	0.53
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.91	0.52
1:A:276:VAL:O	1:A:280:SER:OG	2.26	0.52
1:A:24:TRP:CH2	4:T:704:DG:C8	2.97	0.52
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.44	0.52
2:B:64:LYS:HE2	2:B:68:SER:O	2.09	0.52
1:A:500:GLN:HG2	2:B:422:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LYS:HD2	2:B:405:TYR:CD1	2.44	0.52
2:B:425:LEU:HA	2:B:428:GLN:HG3	1.90	0.52
2:B:195:ILE:HG13	2:B:199:ARG:HH11	1.73	0.52
1:A:63:ILE:HD13	1:A:74:LEU:CD1	2.40	0.51
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.91	0.51
2:B:357:MET:HE2	2:B:359:GLY:HA3	1.91	0.51
1:A:402:TRP:HE3	1:A:403:THR:HG22	1.66	0.51
2:B:58:THR:HG23	2:B:76:ASP:O	2.09	0.51
2:B:355:ALA:O	2:B:356:ARG:HG2	2.10	0.51
1:A:131:THR:CG2	1:A:143:ARG:CD	2.89	0.51
1:A:549:ASP:O	1:A:553:SER:HB2	2.11	0.51
1:A:424:LYS:HE3	1:A:426:TRP:CZ2	2.46	0.51
2:B:101:LYS:O	2:B:236:PRO:HB2	2.11	0.51
4:T:710:DG:H2''	4:T:711:DC:H5'	1.93	0.51
1:A:402:TRP:HZ2	2:B:362:THR:HG21	1.76	0.50
3:P:812:DT:H2''	3:P:813:DT:C5'	2.40	0.50
1:A:53:GLU:OE1	1:A:53:GLU:N	2.34	0.50
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.93	0.50
1:A:93:GLY:C	1:A:94:ILE:HD13	2.37	0.50
1:A:473:THR:O	1:A:477:THR:HG23	2.11	0.50
2:B:342:TYR:HA	2:B:349:LEU:HD13	1.93	0.50
1:A:246:LEU:HD22	1:A:260:LEU:HD12	1.92	0.50
1:A:245:VAL:HG23	1:A:245:VAL:O	2.12	0.49
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.49
2:B:50:ILE:CG2	2:B:145:GLN:HB2	2.43	0.49
1:A:439:THR:HG23	2:B:289:LEU:HD13	1.95	0.49
1:A:75:VAL:HG11	1:A:77:PHE:CE2	2.48	0.49
2:B:74:LEU:HD11	2:B:409:THR:HA	1.94	0.49
2:B:275:LYS:HE3	2:B:305:GLU:OE1	2.12	0.49
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.94	0.49
2:B:195:ILE:O	2:B:195:ILE:HG13	2.12	0.49
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.95	0.48
1:A:286:THR:HG21	1:A:293:ILE:HD13	1.93	0.48
2:B:164:MET:HG2	2:B:182:GLN:OE1	2.12	0.48
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.79	0.48
2:B:195:ILE:CG1	2:B:199:ARG:NH1	2.76	0.48
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.14	0.48
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.23	0.48
2:B:195:ILE:O	2:B:199:ARG:CG	2.61	0.48
1:A:281:LYS:HD3	1:A:281:LYS:HA	1.64	0.47
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:HG21	2:B:289:LEU:CD1	2.45	0.47
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.96	0.47
2:B:86:ASP:OD1	2:B:86:ASP:N	2.30	0.47
1:A:240:THR:HG23	1:A:241:VAL:O	2.14	0.47
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.97	0.47
1:A:24:TRP:CB	1:A:25:PRO:HD2	2.45	0.47
1:A:418:ASN:O	1:A:420:PRO:HD3	2.14	0.47
1:A:388:LYS:HE2	1:A:413:GLU:OE1	2.15	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.97	0.47
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.76	0.46
1:A:54:ASN:O	1:A:143:ARG:NH2	2.42	0.46
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.78	0.46
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.46
2:B:66:LYS:HG2	2:B:67:ASP:N	2.30	0.46
2:B:268:SER:HB3	2:B:274:ILE:HB	1.97	0.46
1:A:79:GLU:OE2	1:A:83:ARG:NH2	2.50	0.45
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.48	0.45
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.51	0.45
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.17	0.45
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.47	0.45
2:B:332:GLN:OE1	2:B:428:GLN:NE2	2.31	0.45
2:B:410:TRP:C	2:B:411:ILE:HG13	2.42	0.45
2:B:357:MET:O	2:B:357:MET:HG3	2.17	0.45
2:B:328:GLU:O	2:B:339:TYR:HA	2.17	0.45
3:P:810:DT:H2''	3:P:811:DG:C8	2.51	0.45
2:B:53:GLU:OE1	2:B:53:GLU:N	2.37	0.45
2:B:201:LYS:O	2:B:204:GLU:HB3	2.16	0.45
2:B:354:TYR:CZ	2:B:356:ARG:HD2	2.53	0.44
3:P:805:DG:N3	3:P:805:DG:H2'	2.32	0.44
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.99	0.44
2:B:195:ILE:HG13	2:B:199:ARG:NH1	2.32	0.44
1:A:412:PRO:HD3	2:B:401:TRP:CH2	2.52	0.44
2:B:396:GLU:H	2:B:396:GLU:HG2	1.62	0.44
1:A:21:VAL:HG12	1:A:59:PRO:HD3	1.99	0.44
1:A:121:ASP:O	1:A:125:ARG:HG3	2.17	0.44
1:A:305:GLU:O	1:A:309:ILE:HG13	2.17	0.44
2:B:206:ARG:O	2:B:210:LEU:HG	2.18	0.44
4:T:706:DG:H2'	4:T:707:DG:C8	2.53	0.44
1:A:281:LYS:HD2	1:A:284:ARG:CD	2.48	0.43
4:T:710:DG:C2'	4:T:711:DC:H5'	2.48	0.43
4:T:716:DA:H2'	4:T:717:DC:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HZ2	1:A:284:ARG:HD3	1.80	0.43
1:A:396:GLU:H	1:A:396:GLU:HG3	1.58	0.43
2:B:167:ILE:HD13	2:B:212:TRP:CE3	2.53	0.43
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.54	0.43
4:T:716:DA:C2'	4:T:717:DC:O4'	2.67	0.43
1:A:150:PRO:HG2	1:A:153:TRP:HB2	2.00	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD1	2.54	0.42
1:A:253:THR:N	1:A:256:ASP:OD1	2.52	0.42
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.01	0.42
2:B:79:GLU:OE1	2:B:83:ARG:NH1	2.52	0.42
1:A:303:LEU:HD12	1:A:303:LEU:O	2.18	0.42
2:B:104:LYS:O	2:B:235:HIS:ND1	2.43	0.42
2:B:143:ARG:HH11	2:B:143:ARG:HD2	1.62	0.42
2:B:154:LYS:C	2:B:157:PRO:HD2	2.44	0.42
2:B:263:LYS:HA	2:B:426:TRP:CZ3	2.54	0.42
1:A:253:THR:HA	1:A:292:VAL:HA	2.02	0.42
2:B:308:GLU:CD	2:B:311:LYS:HE3	2.44	0.42
1:A:186:ASP:O	1:A:187:LEU:HD23	2.20	0.42
1:A:298:GLU:H	1:A:298:GLU:HG2	1.58	0.42
2:B:173:LYS:HB3	2:B:173:LYS:HE3	1.87	0.42
2:B:24:TRP:HB2	2:B:25:PRO:HD2	2.02	0.42
2:B:39:THR:HG22	8:B:502:HOH:O	2.20	0.42
1:A:402:TRP:CE3	1:A:403:THR:CG2	2.90	0.42
2:B:254:VAL:CG2	2:B:293:ILE:HD11	2.44	0.42
1:A:54:ASN:HB3	1:A:143:ARG:HH22	1.85	0.42
1:A:132:ILE:HA	1:A:133:PRO:HD2	1.54	0.42
1:A:314:VAL:HG22	1:A:315:HIS:N	2.35	0.42
2:B:118:VAL:HG12	2:B:119:PRO:O	2.20	0.42
3:P:810:DT:H2''	3:P:811:DG:H8	1.85	0.42
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.41
2:B:332:GLN:OE1	2:B:428:GLN:HG2	2.20	0.41
2:B:299:ALA:HA	2:B:302:GLU:HG2	2.01	0.41
2:B:239:TRP:CH2	2:B:378:GLU:HA	2.55	0.41
2:B:282:LEU:HD21	2:B:296:THR:HG23	2.02	0.41
2:B:311:LYS:O	2:B:312:GLU:HG3	2.20	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.84	0.41
4:T:711:DC:H2'	4:T:712:DC:H6	1.84	0.41
2:B:422:LEU:HD23	2:B:422:LEU:HA	1.88	0.41
1:A:24:TRP:HH2	1:A:61:PHE:CD1	2.38	0.41
2:B:154:LYS:O	2:B:157:PRO:HD2	2.21	0.41
2:B:354:TYR:CE2	2:B:356:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HD2	1:A:284:ARG:NE	2.36	0.41
1:A:281:LYS:O	1:A:284:ARG:HG3	2.21	0.40
1:A:500:GLN:HG2	2:B:422:LEU:CD1	2.51	0.40
1:A:8:VAL:HA	1:A:9:PRO:HD3	1.81	0.40
1:A:430:GLU:HB2	1:A:532:TYR:HB2	2.04	0.40
2:B:156:SER:N	2:B:157:PRO:HD2	2.36	0.40
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.23	0.40
2:B:10:VAL:HA	8:B:501:HOH:O	2.21	0.40
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.76	0.40
1:A:337:TRP:CD1	1:A:337:TRP:N	2.89	0.40
3:P:815:DG:H2''	3:P:816:DG:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/572 (96%)	522 (95%)	23 (4%)	4 (1%)	18	25
2	B	393/440 (89%)	374 (95%)	19 (5%)	0	100	100
All	All	942/1012 (93%)	896 (95%)	42 (4%)	4 (0%)	30	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	418	ASN
1	A	140	PRO
1	A	412	PRO

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	493/511 (96%)	455 (92%)	38 (8%)	12	17
2	B	362/400 (90%)	344 (95%)	18 (5%)	22	33
All	All	855/911 (94%)	799 (94%)	56 (6%)	15	22

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

Mol	Chain	Res	Type
1	A	16	MET
1	A	24	TRP
1	A	32	LYS
1	A	43	LYS
1	A	63	ILE
1	A	102	LYS
1	A	122	GLU
1	A	132	ILE
1	A	179	VAL
1	A	184	MET
1	A	195	ILE
1	A	200	THR
1	A	211	ARG
1	A	221	HIS
1	A	228	LEU
1	A	240	THR
1	A	241	VAL
1	A	248	GLU
1	A	280	SER
1	A	281	LYS
1	A	293	ILE
1	A	295	LEU
1	A	298	GLU
1	A	338	THR
1	A	340	GLN
1	A	353	LYS
1	A	373	GLN

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Mol	Chain	Res	Type
1	A	393	ILE
1	A	394	GLN
1	A	396	GLU
1	A	403	THR
1	A	418	ASN
1	A	452	LEU
1	A	458	VAL
1	A	512	GLN
1	A	523	GLU
1	A	547	GLN
1	A	553	SER
2	B	10	VAL
2	B	74	LEU
2	B	79	GLU
2	B	86	ASP
2	B	163	SER
2	B	168	LEU
2	B	174	GLN
2	B	187	LEU
2	B	206	ARG
2	B	232	TYR
2	B	241	VAL
2	B	245	VAL
2	B	302	GLU
2	B	315	HIS
2	B	358	ARG
2	B	362	THR
2	B	386	THR
2	B	418	ASN

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

Mol	Chain	Res	Type
1	A	315	HIS
1	A	428	GLN
1	A	487	GLN
1	A	519	ASN
1	A	539	HIS
2	B	137	ASN
2	B	269	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
3	DOC	P	822	4,3	16,19,20	2.20	8 (50%)	20,26,29	3.31	5 (25%)

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
3	DOC	P	822	4,3	-	0/7/18/19	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	DOC	C4-N3	4.16	1.42	1.34
3	P	822	DOC	C5-C4	-3.97	1.33	1.42
3	P	822	DOC	C4-N4	3.45	1.42	1.33
3	P	822	DOC	O4'-C1'	2.56	1.48	1.42
3	P	822	DOC	C6-C5	2.42	1.40	1.35
3	P	822	DOC	C1'-N1	-2.16	1.42	1.48
3	P	822	DOC	O5'-C5'	-2.15	1.37	1.44
3	P	822	DOC	C3'-C2'	-2.07	1.48	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	C2'-C1'-N1	11.82	134.81	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	822	DOC	O4'-C4'-C5'	5.53	119.31	109.34
3	P	822	DOC	C4'-O4'-C1'	-4.65	105.42	109.81
3	P	822	DOC	O4'-C4'-C3'	2.41	108.77	104.81
3	P	822	DOC	O2-C2-N3	-2.19	118.87	122.33

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 oligosaccharides 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	SO4	A	602	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	A	601	-	4,4,4	0.27	0	6,6,6	0.38	0
7	N8G	A	604	6	28,29,29	1.63	5 (17%)	40,45,45	2.09	11 (27%)

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
7	N8G	A	604	6	-	4/22/31/31	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	604	N8G	CAT-CAU	4.41	1.46	1.42
7	A	604	N8G	PAZ-OAG	3.71	1.62	1.50
7	A	604	N8G	PBA-OAR	3.27	1.63	1.59
7	A	604	N8G	PBB-OAE	3.12	1.61	1.50
7	A	604	N8G	CAT-NAN	-2.11	1.30	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604	N8G	FAJ-CAU-CAK	6.74	126.69	120.99
7	A	604	N8G	FAJ-CAU-CAT	-5.56	114.55	118.09
7	A	604	N8G	CAU-CAT-NAA	-5.34	116.38	120.79
7	A	604	N8G	OAI-PBB-OAR	2.87	115.02	107.27
7	A	604	N8G	OAC-PAZ-OAQ	2.85	114.19	104.64
7	A	604	N8G	OAR-PBB-OAE	-2.42	103.43	110.70
7	A	604	N8G	NAA-CAT-NAN	2.29	122.66	118.51
7	A	604	N8G	CAU-CAT-NAN	2.10	120.96	119.59
7	A	604	N8G	CAK-CAU-CAT	-2.06	118.77	120.25
7	A	604	N8G	OAP-CAX-CAM	2.04	113.66	109.26
7	A	604	N8G	OAF-PAZ-OAG	-2.03	102.93	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

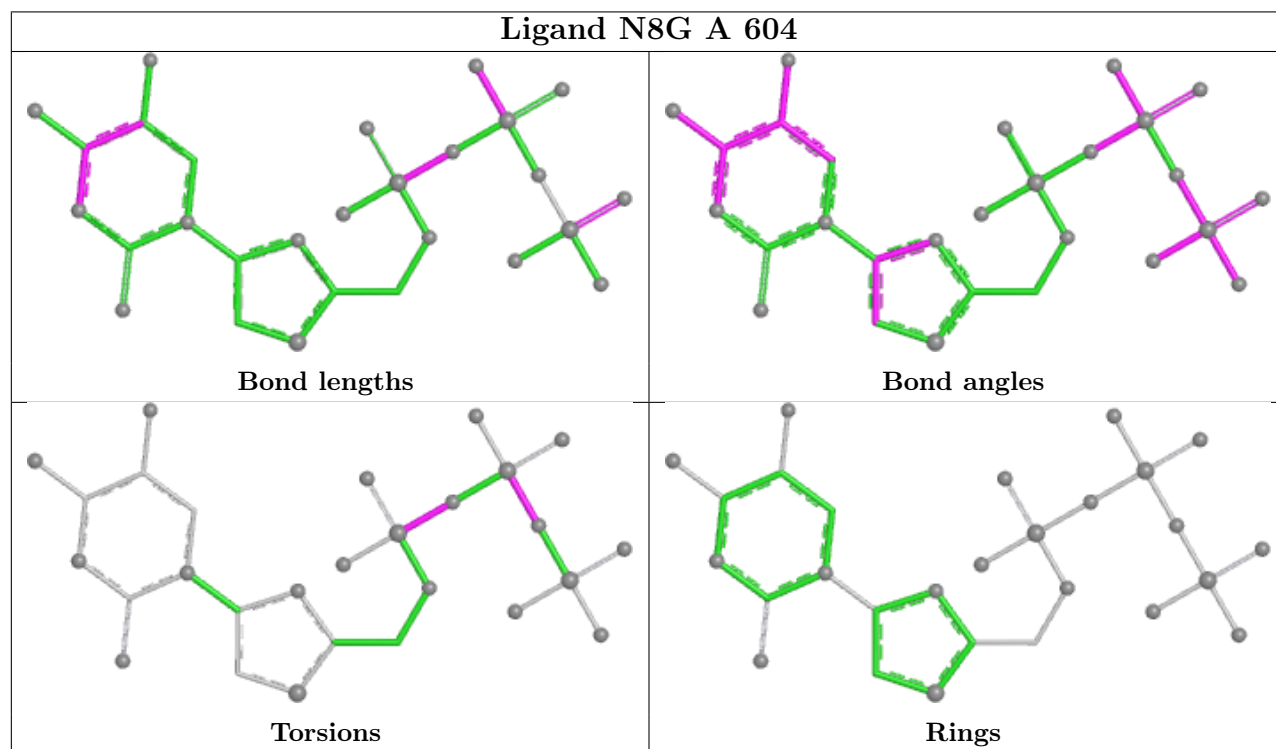
Mol	Chain	Res	Type	Atoms
7	A	604	N8G	PAZ-OAQ-PBB-OAI
7	A	604	N8G	PBB-OAR-PBA-OAD
7	A	604	N8G	PAZ-OAQ-PBB-OAE
7	A	604	N8G	PBB-OAR-PBA-OAH

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	553/572 (96%)	0.04	7 (1%) 75 76	38, 56, 86, 105	0
2	B	399/440 (90%)	0.26	15 (3%) 44 45	39, 64, 92, 114	0
3	P	17/21 (80%)	-0.37	0 100 100	48, 67, 79, 81	0
4	T	24/27 (88%)	-0.11	0 100 100	48, 75, 97, 114	0
All	All	993/1060 (93%)	0.12	22 (2%) 62 63	38, 60, 90, 114	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95	PRO	3.8
2	B	213	GLY	3.7
2	B	231	GLY	3.6
1	A	134	SER	3.4
2	B	429	LEU	3.3
2	B	240	THR	3.2
1	A	290	THR	3.2
2	B	360	ALA	3.1
2	B	315	HIS	3.0
2	B	419	THR	2.7
2	B	232	TYR	2.6
2	B	358	ARG	2.5
1	A	140	PRO	2.4
2	B	417	VAL	2.3
2	B	425	LEU	2.3
2	B	212	TRP	2.2
1	A	406	TRP	2.2
2	B	420	PRO	2.1
1	A	557	ARG	2.1
2	B	361	HIS	2.1
1	A	1	PRO	2.0
1	A	471	ASP	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
3	DOC	P	822	18/19	0.97	0.07	41,49,52,55	0

6.3 Carbohydrates [i](#)

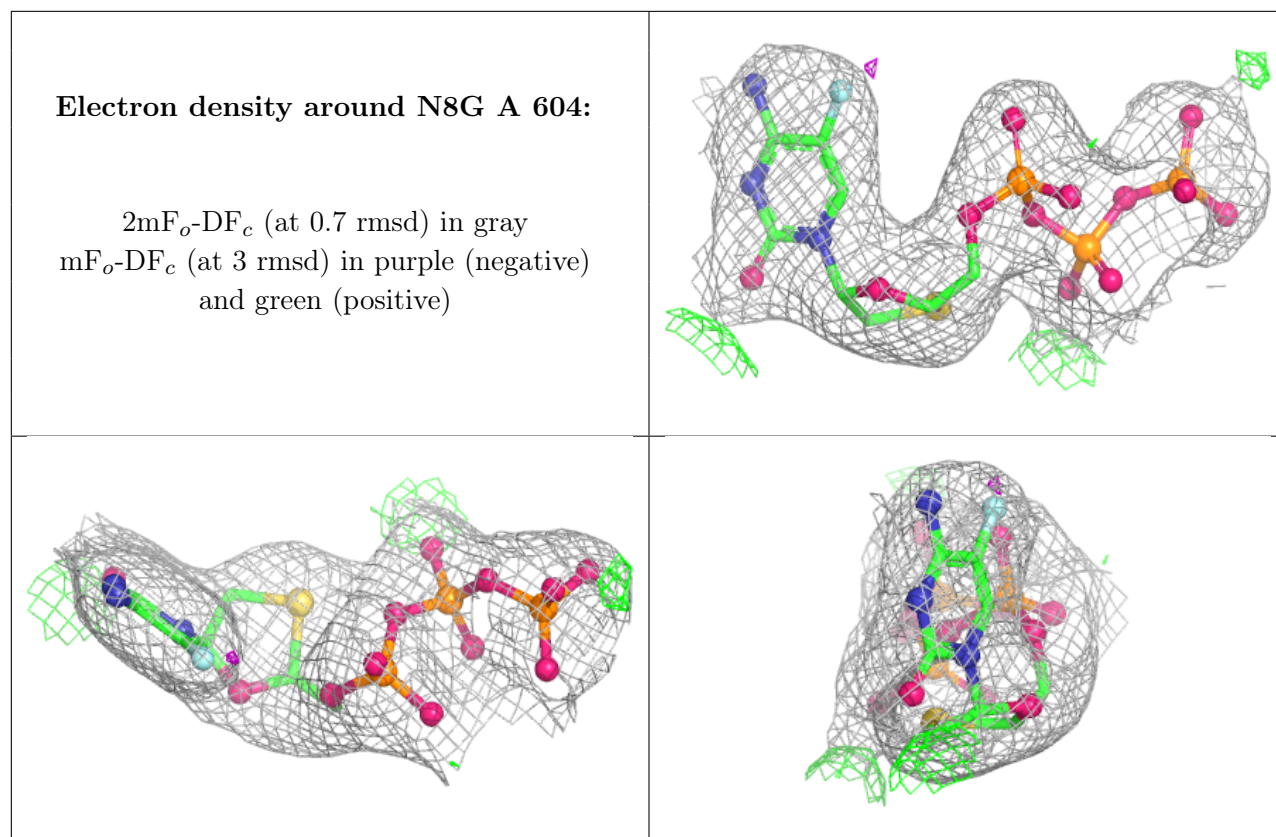
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
5	SO4	A	602	5/5	0.75	0.09	92,95,101,108	0
5	SO4	A	601	5/5	0.97	0.07	58,63,67,68	0
7	N8G	A	604	28/28	0.97	0.06	43,49,58,62	0
6	MG	A	603	1/1	0.99	0.03	41,41,41,41	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.