Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 09:04 PM EDT

PDB ID	:	5I42
Title	:	Structure of HIV-1 Reverse Transcriptase in complex with a DNA aptamer, AZTTP, and CA(2+) ion
Authors	:	Das, K.; Arnold, E.
Deposited on	:	2016-02-11
Resolution	:	3.30 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:

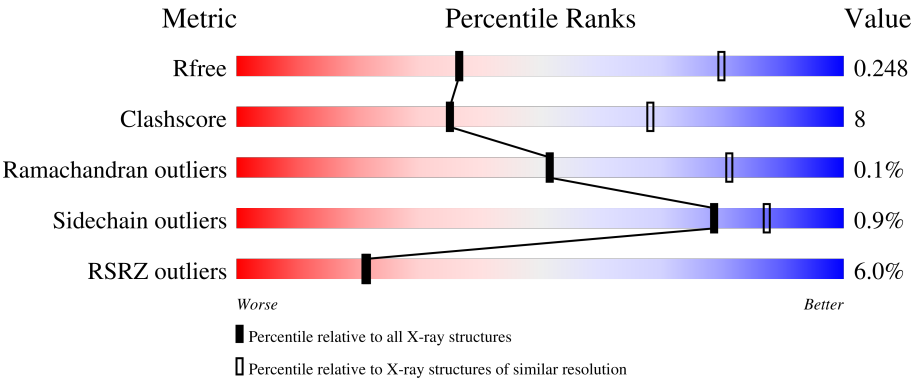
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 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.



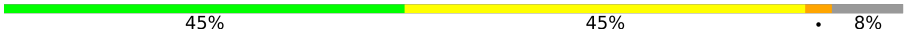
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	555	8% 80% 20%
1	C	555	9% 78% 21%
2	B	444	2% 74% 18% 7%
2	D	444	4% 74% 18% 7%
3	E	38	47% 39% 5% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17320 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4509	2919	750	833	7			
1	C	554	Total	C	N	O	S	0	0	0
			4509	2919	750	833	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3398	2212	562	618	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (38-MER).

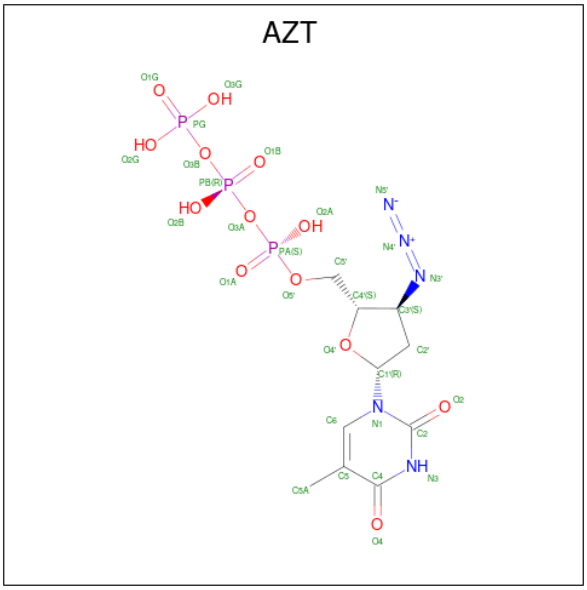
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			
3	F	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			

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

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

- Molecule 5 is 3'-AZIDO-3'-DEOXYTHYMIDINE-5'-TRIPHOSPHATE (three-letter code:

AZT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



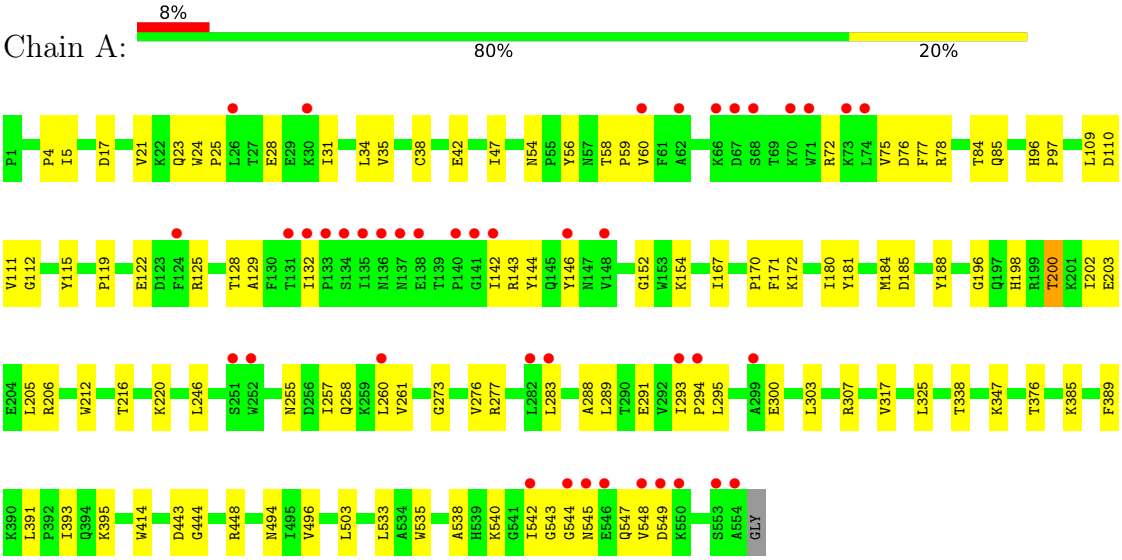
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

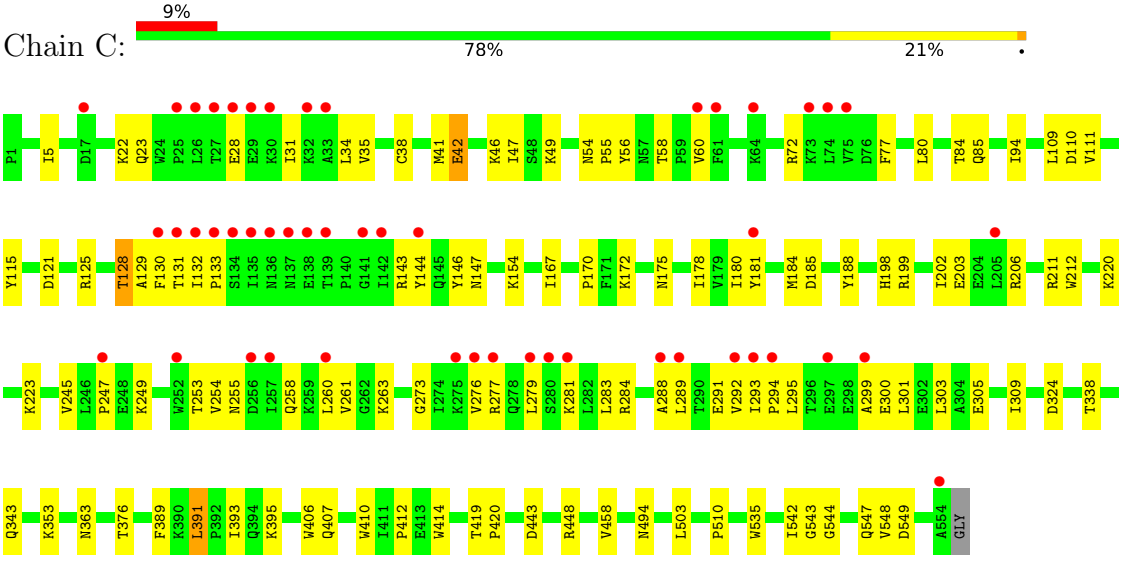
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

Chain A:



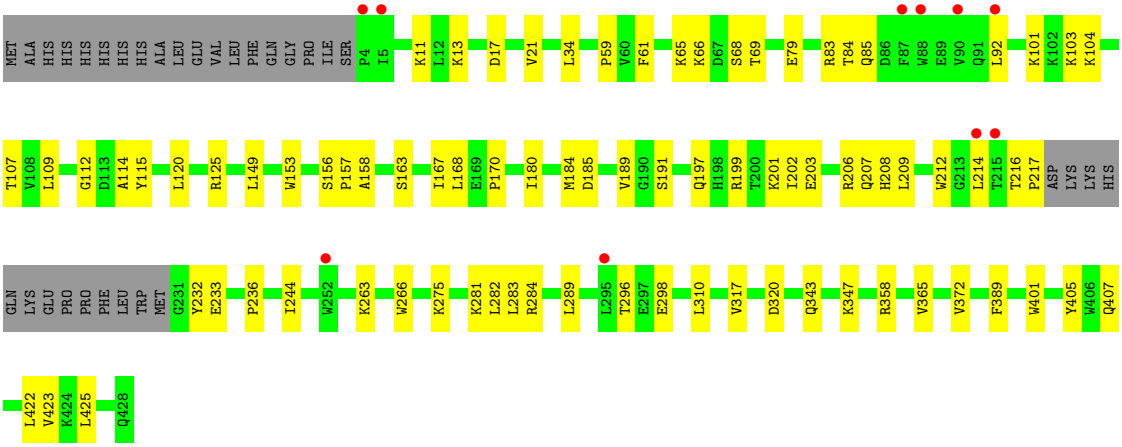
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

Chain C:

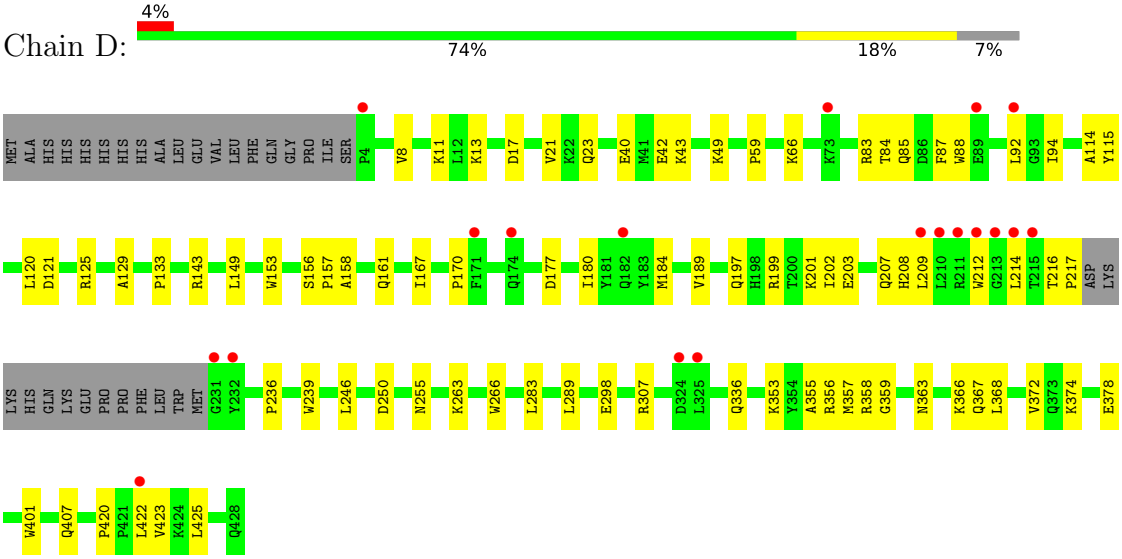


• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT

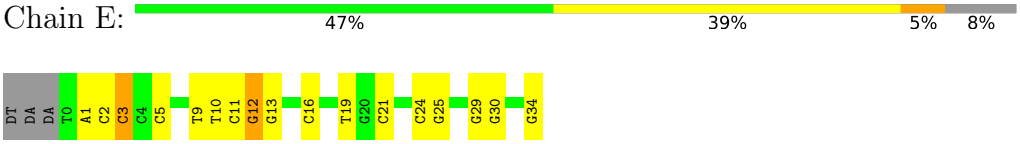
Chain B:



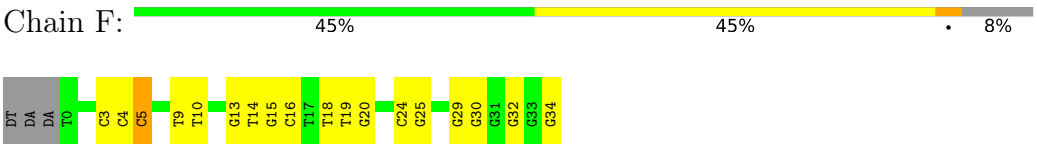
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



• Molecule 3: DNA (38-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.15Å 132.19Å 139.66Å 90.00° 97.15° 90.00°	Depositor
Resolution (Å)	48.45 – 3.30 48.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.45-3.30) 94.5 (48.45-3.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.221 , 0.247 0.221 , 0.248	Depositor DCC
R_{free} test set	1890 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å^2)	105.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17320	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AZT, OMC, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/4627	0.44	0/6286
1	C	0.25	0/4627	0.45	0/6286
2	B	0.26	0/3495	0.44	0/4748
2	D	0.27	0/3497	0.45	0/4751
3	E	0.75	2/759 (0.3%)	1.06	3/1170 (0.3%)
3	F	0.81	1/759 (0.1%)	1.05	2/1170 (0.2%)
All	All	0.33	3/17764 (0.0%)	0.54	5/24411 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	16	DC	C4'-O4'	15.77	1.60	1.45
3	E	16	DC	C4'-O4'	7.06	1.52	1.45
3	E	21	DC	C4'-O4'	5.63	1.50	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	16	DC	O4'-C4'-C3'	-12.41	98.56	106.00
3	F	16	DC	C5'-C4'-O4'	7.64	123.81	109.30
3	E	12	DG	O4'-C4'-C3'	-7.09	101.67	104.50
3	E	12	DG	C5'-C4'-O4'	6.54	121.72	109.30
3	E	21	DC	C5'-C4'-O4'	5.26	119.29	109.30

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	4509	0	4570	78	0
1	C	4509	0	4570	84	0
2	B	3398	0	3431	60	0
2	D	3400	0	3433	56	0
3	E	720	0	397	13	0
3	F	720	0	397	16	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	31	0	12	4	0
5	C	31	0	12	3	0
All	All	17320	0	16822	280	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 8.

All (280) 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:A:255:ASN:HB2	1:A:289:LEU:CD2	2.07	0.85
1:C:34:LEU:HD21	1:C:132:ILE:HD12	1.59	0.83
1:C:448:ARG:HH21	3:F:19:DT:H5"	1.47	0.78
1:A:448:ARG:HH21	3:E:19:DT:H5"	1.48	0.78
1:A:110:ASP:OD2	1:A:111:VAL:N	2.16	0.78
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.67	0.77
1:A:34:LEU:HD21	1:A:132:ILE:HD12	1.67	0.75
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.67	0.74
3:E:24:DC:H2"	3:E:25:DG:C8	2.22	0.74
1:A:255:ASN:HB2	1:A:289:LEU:HD21	1.68	0.73
1:C:128:THR:HG21	1:C:146:TYR:HB2	1.70	0.72
2:B:358:ARG:NH2	2:B:405:TYR:O	2.24	0.70
2:B:206:ARG:NH2	2:B:216:THR:O	2.23	0.70
1:C:255:ASN:OD1	1:C:289:LEU:HD21	1.91	0.70
1:C:84:THR:HB	1:C:154:LYS:HE2	1.74	0.69
2:D:359:GLY:HA3	2:D:366:LYS:HD2	1.74	0.69
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:ILE:HG12	2:D:189:VAL:HG22	1.75	0.68
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.31	0.66
1:A:184:MET:HG2	3:E:34:DG:H2"	1.78	0.66
2:D:66:LYS:HG3	2:D:358:ARG:HH22	1.60	0.65
1:C:255:ASN:HB2	1:C:289:LEU:CD2	2.26	0.65
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.32	0.65
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.79	0.65
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.80	0.63
1:C:203:GLU:OE2	1:C:206:ARG:NH1	2.29	0.63
1:A:255:ASN:HB2	1:A:289:LEU:HD23	1.81	0.63
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.81	0.63
1:C:172:LYS:HE2	1:C:180:ILE:HB	1.81	0.62
1:C:389:PHE:HB3	1:C:391:LEU:HD13	1.82	0.62
1:C:295:LEU:HB3	1:C:300:GLU:HG2	1.82	0.62
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.82	0.61
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.82	0.61
2:B:203:GLU:O	2:B:207:GLN:HG2	2.01	0.60
2:D:358:ARG:NH2	2:D:407:GLN:HE22	1.98	0.60
1:C:94:ILE:HD11	3:F:32:DG:H21	1.65	0.60
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.84	0.60
1:A:54:ASN:O	1:A:143:ARG:NH2	2.34	0.60
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.84	0.60
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.83	0.60
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.65	0.60
1:C:255:ASN:HB2	1:C:289:LEU:HD23	1.83	0.59
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.84	0.59
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.84	0.59
1:A:389:PHE:HB3	1:A:391:LEU:HD13	1.84	0.59
1:A:115:TYR:CE2	5:A:602:AZT:H2'1	2.38	0.59
1:C:254:VAL:HG13	1:C:283:LEU:HD22	1.84	0.58
1:A:47:ILE:HD12	1:A:146:TYR:HA	1.85	0.58
2:D:336:GLN:HG2	2:D:353:LYS:NZ	2.19	0.58
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.85	0.57
1:C:260:LEU:HD21	1:C:303:LEU:HD13	1.86	0.57
2:D:336:GLN:HG3	2:D:355:ALA:HB2	1.87	0.56
1:A:84:THR:HB	1:A:154:LYS:HE2	1.87	0.56
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.86	0.56
2:D:92:LEU:HB3	2:D:158:ALA:HB1	1.87	0.56
1:A:258:GLN:HB3	3:E:30:DG:H4'	1.88	0.56
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.88	0.55
1:C:47:ILE:HD12	1:C:146:TYR:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.87	0.55
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.87	0.55
1:C:115:TYR:CE2	5:C:602:AZT:H2'1	2.41	0.55
2:B:197:GLN:O	2:B:201:LYS:HG2	2.07	0.55
3:F:14:DT:H4'	3:F:15:DG:OP1	2.06	0.55
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.42	0.55
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.89	0.54
2:D:266:TRP:CD1	2:D:425:LEU:HD22	2.42	0.54
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.89	0.54
1:C:54:ASN:O	1:C:143:ARG:NH2	2.41	0.54
2:B:281:LYS:HG2	2:B:284:ARG:HH11	1.72	0.54
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.90	0.54
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.90	0.54
1:A:255:ASN:CB	1:A:289:LEU:HD21	2.38	0.53
2:D:422:LEU:HG	2:D:423:VAL:HG12	1.90	0.53
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.89	0.53
1:C:258:GLN:HB3	3:F:30:DG:H4'	1.91	0.53
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.36	0.53
1:C:543:GLY:HA2	2:D:283:LEU:O	2.09	0.53
2:D:17:ASP:O	2:D:83:ARG:HD3	2.09	0.53
2:B:65:LYS:HB3	2:B:232:TYR:OH	2.09	0.53
1:C:28:GLU:HA	1:C:31:ILE:HD12	1.90	0.52
2:B:320:ASP:O	2:B:343:GLN:NE2	2.37	0.52
1:C:391:LEU:HB3	1:C:393:ILE:HG22	1.90	0.52
1:A:47:ILE:HG13	1:A:144:TYR:HB3	1.92	0.52
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.44	0.52
1:C:35:VAL:HA	1:C:38:CYS:HB3	1.92	0.52
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.73	0.52
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.91	0.52
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.92	0.52
1:C:258:GLN:NE2	3:F:29:DG:H2"	2.24	0.51
1:C:110:ASP:HB3	1:C:220:LYS:HB3	1.91	0.51
2:D:66:LYS:HG3	2:D:358:ARG:NH2	2.25	0.51
1:A:258:GLN:NE2	3:E:29:DG:H2"	2.25	0.51
2:B:17:ASP:O	2:B:83:ARG:HD3	2.10	0.51
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.92	0.51
2:D:209:LEU:HD13	2:D:214:LEU:HD23	1.92	0.51
2:D:336:GLN:HG2	2:D:353:LYS:HZ2	1.74	0.51
2:D:236:PRO:HA	2:D:239:TRP:CE2	2.45	0.51
1:C:47:ILE:HG13	1:C:144:TYR:HB3	1.92	0.51
2:D:246:LEU:HD12	2:D:307:ARG:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ASP:HB2	1:C:548:VAL:HG13	1.92	0.50
2:D:203:GLU:O	2:D:207:GLN:HG2	2.12	0.50
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.94	0.50
2:D:177:ASP:OD1	2:D:177:ASP:N	2.43	0.50
1:A:23:GLN:HE22	1:A:60:VAL:HB	1.76	0.50
1:A:391:LEU:HB3	1:A:393:ILE:HG22	1.94	0.50
2:B:157:PRO:HG3	2:B:184:MET:HA	1.93	0.50
1:A:395:LYS:NZ	1:A:414:TRP:O	2.45	0.49
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.46	0.49
1:A:543:GLY:HA2	2:B:283:LEU:O	2.12	0.49
1:C:253:THR:HA	1:C:292:VAL:HA	1.95	0.49
2:B:17:ASP:O	2:B:83:ARG:NH1	2.45	0.49
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.48	0.49
2:D:157:PRO:HG3	2:D:184:MET:HA	1.94	0.49
3:E:12:DG:H1'	3:E:13:DG:C8	2.48	0.49
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.48	0.49
1:A:28:GLU:HA	1:A:31:ILE:HD12	1.95	0.48
1:A:35:VAL:HA	1:A:38:CYS:HB3	1.95	0.48
2:B:263:LYS:HA	2:B:423:VAL:HG21	1.95	0.48
1:C:199:ARG:CZ	1:C:223:LYS:HD3	2.42	0.48
2:D:40:GLU:HA	2:D:43:LYS:HG2	1.94	0.48
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.95	0.48
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.94	0.48
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.95	0.48
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.12	0.48
1:C:31:ILE:HD13	1:C:133:PRO:HB2	1.95	0.48
3:F:19:DT:H4'	3:F:20:DG:O5'	2.14	0.48
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.48	0.48
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.95	0.48
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.48	0.48
1:A:544:GLY:HA2	1:A:547:GLN:HG2	1.95	0.48
2:B:199:ARG:NE	2:B:233:GLU:OE2	2.47	0.48
2:D:266:TRP:HD1	2:D:425:LEU:HD22	1.78	0.48
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.96	0.48
3:F:4:DC:H2'	3:F:5:OMC:C6	2.49	0.48
1:A:258:GLN:HB3	3:E:30:DG:C4'	2.44	0.47
1:C:443:ASP:OD2	1:C:549:ASP:HA	2.14	0.47
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.96	0.47
2:D:197:GLN:O	2:D:201:LYS:HG2	2.14	0.47
1:C:42:GLU:OE1	1:C:49:LYS:HE3	2.14	0.47
1:C:72:ARG:HH22	5:C:602:AZT:PA	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:24:DC:H2"	3:F:25:DG:C8	2.49	0.47
1:A:325:LEU:HD12	1:A:385:LYS:HG3	1.97	0.47
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.47
2:B:281:LYS:HA	2:B:284:ARG:HD3	1.95	0.47
1:C:247:PRO:HB3	1:C:249:LYS:NZ	2.30	0.47
1:C:110:ASP:OD2	1:C:111:VAL:N	2.48	0.47
1:C:363:ASN:HB3	1:C:510:PRO:HA	1.97	0.47
2:D:167:ILE:HG23	2:D:212:TRP:CD1	2.50	0.47
1:A:60:VAL:HG22	1:A:75:VAL:HG22	1.97	0.46
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.97	0.46
2:D:13:LYS:HD2	2:D:85:GLN:HB3	1.95	0.46
2:D:167:ILE:HG12	2:D:212:TRP:CD2	2.51	0.46
2:D:263:LYS:HA	2:D:423:VAL:HG21	1.97	0.46
1:A:58:THR:HG21	1:A:77:PHE:HE1	1.79	0.46
1:C:276:VAL:HG23	1:C:353:LYS:HE2	1.97	0.46
1:C:458:VAL:HG23	1:C:548:VAL:HB	1.97	0.46
1:C:80:LEU:O	1:C:84:THR:OG1	2.29	0.46
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.80	0.46
1:C:121:ASP:O	1:C:125:ARG:HG3	2.16	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.46
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.81	0.46
2:B:275:LYS:HA	2:B:275:LYS:HD3	1.77	0.46
1:C:115:TYR:CD2	5:C:602:AZT:H2'1	2.50	0.46
2:D:363:ASN:O	2:D:367:GLN:HG3	2.16	0.46
1:C:22:LYS:HD3	1:C:22:LYS:HA	1.69	0.46
3:F:9:DT:H2"	3:F:10:DT:O5'	2.16	0.46
1:C:289:LEU:HD12	3:F:29:DG:H4'	1.97	0.46
2:B:298:GLU:CD	2:B:298:GLU:H	2.19	0.46
1:A:206:ARG:NH2	1:A:216:THR:O	2.50	0.45
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.97	0.45
1:A:258:GLN:OE1	3:E:30:DG:H5'	2.17	0.45
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.51	0.45
1:A:142:ILE:HB	1:A:144:TYR:CZ	2.50	0.45
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.45
2:D:23:GLN:HG2	2:D:133:PRO:HD3	1.98	0.45
1:C:23:GLN:HG3	1:C:131:THR:HG22	1.99	0.45
1:A:112:GLY:HA2	5:A:602:AZT:O1G	2.17	0.45
1:A:496:VAL:HG21	2:B:289:LEU:HD21	1.98	0.45
1:A:255:ASN:OD1	1:A:289:LEU:HD21	2.17	0.45
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.68	0.45
1:A:110:ASP:OD2	1:A:110:ASP:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:HA	1:A:125:ARG:NH1	2.31	0.45
1:C:376:THR:HG21	2:D:401:TRP:CH2	2.52	0.45
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.98	0.45
1:C:58:THR:HG21	1:C:77:PHE:HE1	1.81	0.44
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.81	0.44
1:C:395:LYS:NZ	1:C:414:TRP:O	2.50	0.44
2:D:368:LEU:O	2:D:372:VAL:HG23	2.17	0.44
3:E:2:DC:H2'	3:E:3:OMC:C6	2.52	0.44
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.98	0.44
1:A:258:GLN:CD	3:E:29:DG:H2"	2.38	0.44
3:E:11:DC:H2"	3:E:12:DG:C8	2.53	0.44
3:F:5:OMC:HM23	3:F:5:OMC:H1'	1.73	0.44
2:D:8:VAL:O	2:D:121:ASP:HB2	2.18	0.44
1:C:167:ILE:O	1:C:170:PRO:HD2	2.17	0.44
1:C:175:ASN:HB3	1:C:178:ILE:HG12	1.98	0.44
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.82	0.44
2:B:184:MET:HB3	2:B:185:ASP:H	1.64	0.44
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.98	0.44
1:C:184:MET:HG2	3:F:34:DG:H2"	2.00	0.44
2:B:65:LYS:HB2	2:B:68:SER:HB2	2.00	0.44
2:B:65:LYS:HE2	2:B:232:TYR:OH	2.18	0.43
1:A:115:TYR:CD2	5:A:602:AZT:H2'1	2.53	0.43
1:A:171:PHE:CG	1:A:205:LEU:HD13	2.52	0.43
1:A:196:GLY:O	1:A:200:THR:OG1	2.36	0.43
2:B:281:LYS:HG2	2:B:284:ARG:NH1	2.32	0.43
1:C:494:ASN:HB3	2:D:289:LEU:HD12	2.00	0.43
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.53	0.43
2:B:104:LYS:HE2	2:B:104:LYS:HB3	1.78	0.43
2:B:107:THR:HA	2:B:232:TYR:O	2.19	0.43
1:C:94:ILE:HD11	3:F:32:DG:N2	2.31	0.43
1:C:542:ILE:HG23	2:D:283:LEU:HD13	2.00	0.43
2:D:298:GLU:CD	2:D:298:GLU:H	2.21	0.43
2:D:84:THR:HG22	2:D:87:PHE:HB3	2.01	0.43
1:A:72:ARG:HH22	5:A:602:AZT:PA	2.42	0.43
1:A:167:ILE:O	1:A:170:PRO:HD2	2.19	0.43
2:B:34:LEU:HD11	2:B:61:PHE:HA	2.01	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.43
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.84	0.43
1:C:544:GLY:HA2	1:C:547:GLN:HG2	2.01	0.42
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.54	0.42
2:D:255:ASN:HB2	2:D:289:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:13:DG:H2'	3:F:14:DT:H71	2.01	0.42
1:C:23:GLN:HG3	1:C:131:THR:CG2	2.49	0.42
1:A:132:ILE:HD13	1:A:132:ILE:HA	1.90	0.42
1:A:494:ASN:HB3	2:B:289:LEU:HD12	2.02	0.42
1:C:211:ARG:HB2	1:C:212:TRP:CE3	2.54	0.42
2:D:357:MET:HG3	2:D:358:ARG:H	1.84	0.42
3:E:9:DT:H2'	3:E:10:DT:H71	2.00	0.42
1:A:260:LEU:HD21	1:A:303:LEU:HD13	2.01	0.42
2:B:216:THR:HA	2:B:217:PRO:HD2	1.89	0.42
1:C:58:THR:HG22	1:C:129:ALA:O	2.19	0.42
1:C:245:VAL:O	1:C:263:LYS:NZ	2.52	0.42
1:A:24:TRP:HE3	1:A:25:PRO:HD2	1.84	0.42
1:C:301:LEU:O	1:C:305:GLU:HG2	2.20	0.42
2:D:216:THR:HA	2:D:217:PRO:HD2	1.87	0.42
1:C:254:VAL:O	1:C:258:GLN:HG3	2.20	0.42
1:A:129:ALA:HA	1:A:144:TYR:O	2.19	0.42
1:C:293:ILE:HG13	1:C:294:PRO:HD2	2.02	0.42
1:C:305:GLU:O	1:C:309:ILE:HG13	2.20	0.42
1:A:4:PRO:HG2	1:A:119:PRO:HD3	2.02	0.41
1:A:172:LYS:HE2	1:A:180:ILE:HB	2.01	0.41
1:A:293:ILE:HG13	1:A:294:PRO:HD2	2.02	0.41
2:B:103:LYS:HD2	2:B:191:SER:HA	2.02	0.41
2:B:163:SER:O	2:B:167:ILE:HG13	2.20	0.41
3:F:18:DT:H1'	3:F:20:DG:C2	2.56	0.41
1:A:152:GLY:HA2	3:E:1:DA:N3	2.35	0.41
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.00	0.41
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.55	0.41
1:C:125:ARG:HE	1:C:147:ASN:HA	1.86	0.41
1:C:198:HIS:O	1:C:202:ILE:HG12	2.20	0.41
2:B:66:LYS:HG2	2:B:407:GLN:OE1	2.20	0.41
2:B:109:LEU:HD11	2:B:202:ILE:HG23	2.02	0.41
2:B:422:LEU:HG	2:B:423:VAL:HG12	2.02	0.41
1:C:42:GLU:HG2	1:C:47:ILE:HG22	2.03	0.41
1:C:419:THR:HA	1:C:420:PRO:HD3	1.86	0.41
2:D:422:LEU:HG	2:D:423:VAL:N	2.36	0.41
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.85	0.41
1:C:261:VAL:HG13	1:C:276:VAL:HG11	2.03	0.41
1:A:295:LEU:HB3	1:A:300:GLU:HG2	2.02	0.41
2:B:112:GLY:HA2	2:B:115:TYR:CD1	2.56	0.41
2:B:115:TYR:O	2:B:149:LEU:HB2	2.21	0.41
2:B:317:VAL:HG12	2:B:347:LYS:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HA	1:C:133:PRO:HD3	1.93	0.41
2:D:94:ILE:HG12	2:D:161:GLN:NE2	2.36	0.41
2:D:374:LYS:O	2:D:378:GLU:HG3	2.20	0.41
1:A:58:THR:HG22	1:A:129:ALA:O	2.20	0.41
1:C:412:PRO:HD3	2:D:401:TRP:CZ2	2.55	0.41
2:D:129:ALA:HB1	2:D:143:ARG:NH2	2.36	0.41
1:C:281:LYS:O	1:C:284:ARG:HG2	2.22	0.40
2:D:115:TYR:O	2:D:149:LEU:HB2	2.21	0.40
2:D:336:GLN:HG3	2:D:355:ALA:CB	2.50	0.40
2:B:101:LYS:O	2:B:236:PRO:HB2	2.21	0.40
1:C:258:GLN:HB3	3:F:30:DG:C4'	2.51	0.40
1:C:324:ASP:O	1:C:343:GLN:HG2	2.22	0.40
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.56	0.40
2:B:68:SER:O	2:B:69:THR:HB	2.22	0.40
1:C:406:TRP:CD1	1:C:407:GLN:HG3	2.56	0.40
1:A:545:ASN:O	1:A:549:ASP:HB2	2.22	0.40
2:B:168:LEU:HD22	2:B:180:ILE:HD13	2.04	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	552/555 (100%)	532 (96%)	20 (4%)	0	100 100
1	C	552/555 (100%)	532 (96%)	19 (3%)	1 (0%)	47 77
2	B	408/444 (92%)	395 (97%)	13 (3%)	0	100 100
2	D	408/444 (92%)	394 (97%)	14 (3%)	0	100 100
All	All	1920/1998 (96%)	1853 (96%)	66 (3%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	PRO

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	495/495 (100%)	489 (99%)	6 (1%)	71	83
1	C	495/495 (100%)	489 (99%)	6 (1%)	71	83
2	B	373/403 (93%)	372 (100%)	1 (0%)	92	96
2	D	374/403 (93%)	371 (99%)	3 (1%)	81	89
All	All	1737/1796 (97%)	1721 (99%)	16 (1%)	78	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	42	GLU
1	A	85	GLN
1	A	109	LEU
1	A	200	THR
1	A	277	ARG
2	B	11	LYS
1	C	42	GLU
1	C	85	GLN
1	C	109	LEU
1	C	128	THR
1	C	277	ARG
1	C	391	LEU
2	D	11	LYS
2	D	250	ASP
2	D	356	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
2	B	208	HIS
1	C	373	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	$\#\|Z\| > 2$
3	OMC	F	5	3	19,22,23	2.71	6 (31%)	26,31,34	0.72	0
3	OMC	F	3	3	19,22,23	2.72	6 (31%)	26,31,34	0.77	0
3	OMC	E	5	3	19,22,23	2.70	6 (31%)	26,31,34	0.73	0
3	OMC	E	3	3	19,22,23	2.71	6 (31%)	26,31,34	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	5	3	-	1/9/27/28	0/2/2/2
3	OMC	F	3	3	-	0/9/27/28	0/2/2/2
3	OMC	E	5	3	-	0/9/27/28	0/2/2/2
3	OMC	E	3	3	-	1/9/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	OMC	C6-C5	6.03	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	OMC	C6-C5	5.98	1.49	1.35
3	E	3	OMC	C6-C5	5.97	1.48	1.35
3	F	5	OMC	C6-C5	5.97	1.48	1.35
3	E	3	OMC	C2-N3	5.79	1.48	1.36
3	F	5	OMC	C2-N3	5.77	1.48	1.36
3	F	3	OMC	C2-N3	5.76	1.48	1.36
3	E	5	OMC	C2-N3	5.72	1.48	1.36
3	E	3	OMC	C4-N3	5.34	1.45	1.34
3	F	3	OMC	C4-N3	5.32	1.45	1.34
3	F	5	OMC	C4-N3	5.31	1.45	1.34
3	E	5	OMC	C4-N3	5.30	1.45	1.34
3	F	3	OMC	C2-N1	4.11	1.48	1.40
3	F	5	OMC	C2-N1	4.04	1.48	1.40
3	E	3	OMC	C2-N1	4.01	1.48	1.40
3	E	5	OMC	C2-N1	3.97	1.48	1.40
3	E	5	OMC	C4-N4	3.42	1.41	1.33
3	F	5	OMC	C4-N4	3.39	1.41	1.33
3	E	3	OMC	C4-N4	3.37	1.41	1.33
3	F	3	OMC	C4-N4	3.34	1.41	1.33
3	F	3	OMC	C6-N1	3.17	1.45	1.38
3	F	5	OMC	C6-N1	3.09	1.45	1.38
3	E	3	OMC	C6-N1	3.07	1.45	1.38
3	E	5	OMC	C6-N1	3.04	1.45	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	OMC	C1'-C2'-O2'-CM2
3	F	5	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	OMC	2	0
3	E	3	OMC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	AZT	A	602	4	27,32,32	2.96	8 (29%)	40,49,49	2.13	15 (37%)
5	AZT	C	602	4	27,32,32	3.01	8 (29%)	40,49,49	2.13	15 (37%)

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	AZT	A	602	4	-	6/25/37/37	0/2/2/2
5	AZT	C	602	4	-	6/25/37/37	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	AZT	O4-C4	9.67	1.42	1.23
5	A	602	AZT	O4-C4	9.58	1.41	1.23
5	C	602	AZT	O2-C2	8.64	1.38	1.23
5	A	602	AZT	O2-C2	8.59	1.38	1.23
5	C	602	AZT	C6-C5	4.98	1.42	1.34
5	A	602	AZT	C6-C5	4.77	1.42	1.34
5	C	602	AZT	C4-N3	3.09	1.44	1.38
5	A	602	AZT	C4-N3	3.07	1.44	1.38
5	C	602	AZT	C2-N3	2.95	1.43	1.38
5	C	602	AZT	C6-N1	2.92	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	AZT	C2-N3	2.89	1.43	1.38
5	C	602	AZT	C2-N1	2.86	1.43	1.38
5	A	602	AZT	C2-N1	2.81	1.43	1.38
5	A	602	AZT	C6-N1	2.80	1.42	1.38
5	C	602	AZT	C3'-N3'	-2.30	1.42	1.48
5	A	602	AZT	C3'-N3'	-2.10	1.42	1.48

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	AZT	C4-N3-C2	-5.63	120.06	127.35
5	C	602	AZT	C4-N3-C2	-5.47	120.27	127.35
5	A	602	AZT	C5-C4-N3	4.89	119.49	115.31
5	C	602	AZT	C5-C4-N3	4.42	119.09	115.31
5	A	602	AZT	O4-C4-C5	-3.97	120.30	124.90
5	C	602	AZT	N3-C2-N1	3.90	120.06	114.89
5	C	602	AZT	O4-C4-C5	-3.82	120.48	124.90
5	A	602	AZT	N3-C2-N1	3.68	119.77	114.89
5	C	602	AZT	PB-O3B-PG	-3.48	120.90	132.83
5	A	602	AZT	PB-O3B-PG	-3.42	121.09	132.83
5	C	602	AZT	PB-O3A-PA	-2.98	122.59	132.83
5	A	602	AZT	PB-O3A-PA	-2.90	122.88	132.83
5	A	602	AZT	C5-C6-N1	-2.89	120.36	123.34
5	C	602	AZT	O3G-PG-O3B	2.88	114.29	104.64
5	C	602	AZT	O2G-PG-O3B	2.88	114.29	104.64
5	A	602	AZT	O3G-PG-O3B	2.86	114.22	104.64
5	C	602	AZT	C5-C6-N1	-2.76	120.50	123.34
5	C	602	AZT	C6-C5-C4	2.75	120.33	118.03
5	C	602	AZT	O4'-C1'-N1	2.75	112.78	107.86
5	A	602	AZT	O2G-PG-O3B	2.62	113.42	104.64
5	A	602	AZT	C6-C5-C4	2.46	120.09	118.03
5	C	602	AZT	C5A-C5-C6	-2.33	119.73	122.85
5	C	602	AZT	O2A-PA-O1A	-2.32	100.78	112.24
5	A	602	AZT	C5A-C5-C6	-2.28	119.81	122.85
5	A	602	AZT	C3'-C2'-C1'	2.24	105.65	103.25
5	A	602	AZT	O2A-PA-O1A	-2.23	101.23	112.24
5	C	602	AZT	O2B-PB-O1B	-2.17	101.52	112.24
5	A	602	AZT	O2B-PB-O1B	-2.16	101.56	112.24
5	A	602	AZT	O4'-C1'-N1	2.05	111.53	107.86
5	C	602	AZT	O2-C2-N1	-2.05	120.07	122.79

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	AZT	C5'-O5'-PA-O1A
5	A	602	AZT	C5'-O5'-PA-O2A
5	C	602	AZT	C5'-O5'-PA-O1A
5	C	602	AZT	C4'-C3'-N3'-N4'
5	A	602	AZT	C2'-C3'-N3'-N4'
5	A	602	AZT	C4'-C3'-N3'-N4'
5	A	602	AZT	PB-O3A-PA-O5'
5	C	602	AZT	PB-O3A-PA-O5'
5	A	602	AZT	C5'-O5'-PA-O3A
5	C	602	AZT	C5'-O5'-PA-O3A
5	C	602	AZT	C5'-O5'-PA-O2A
5	C	602	AZT	C2'-C3'-N3'-N4'

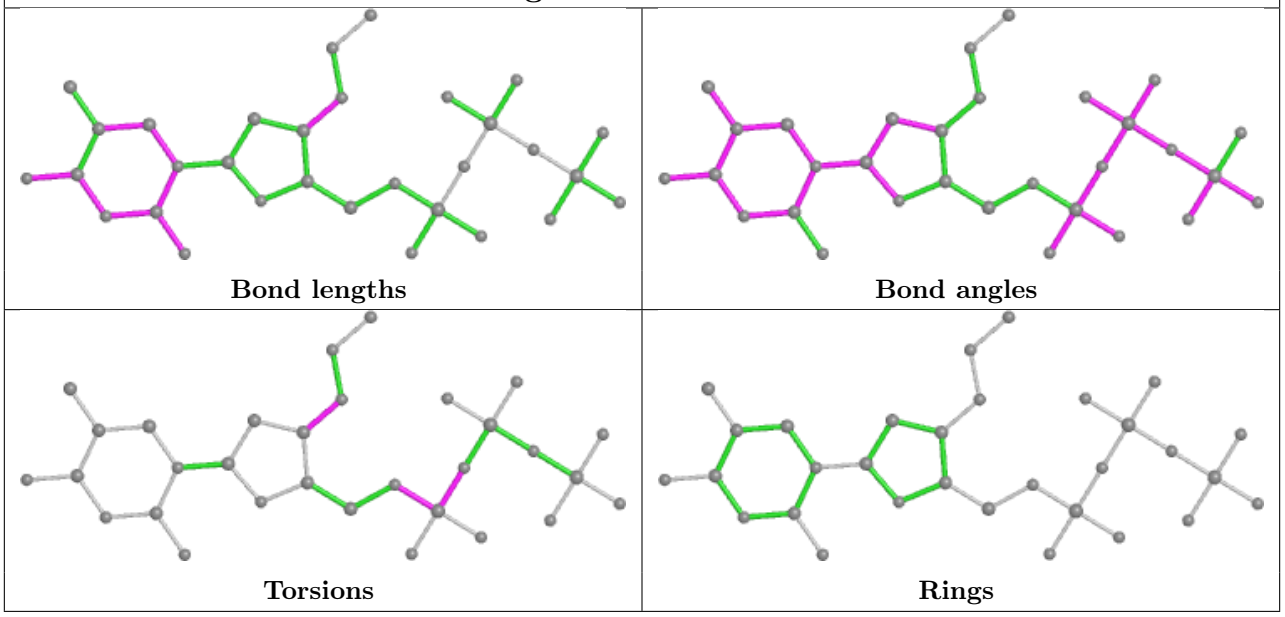
There are no ring outliers.

2 monomers are involved in 7 short contacts:

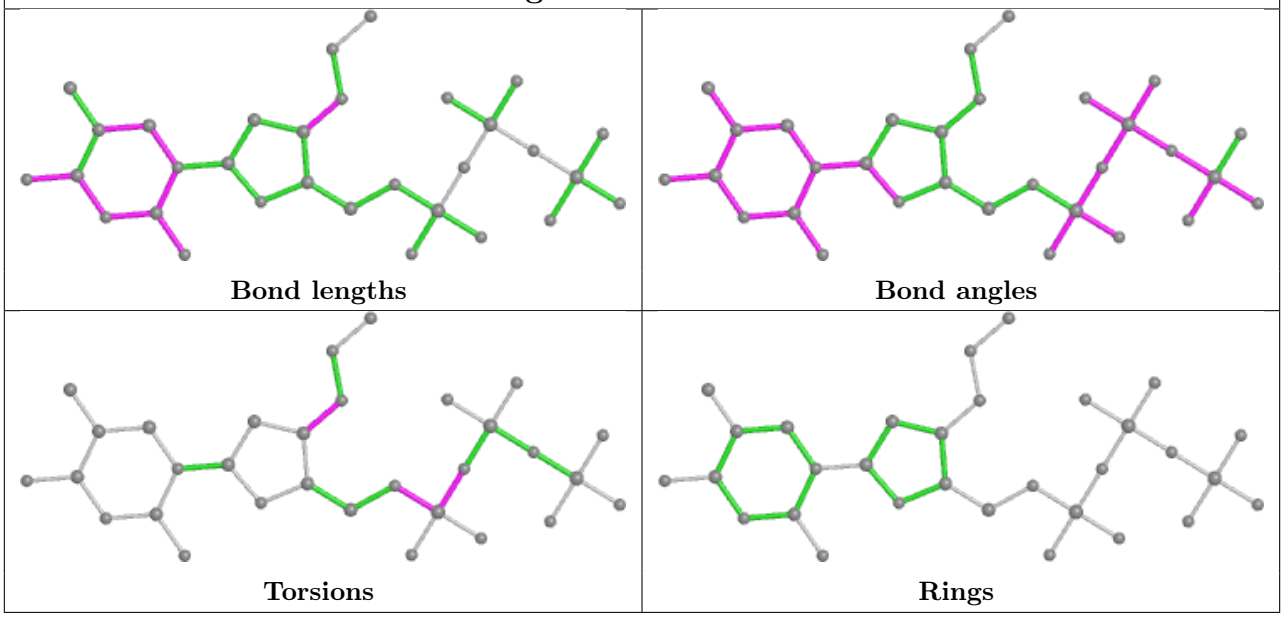
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	AZT	4	0
5	C	602	AZT	3	0

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 then 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.

Ligand AZT A 602



Ligand AZT C 602



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, 95^{th} 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	554/555 (99%)	0.34	42 (7%) 13 13	56, 111, 172, 201	0
1	C	554/555 (99%)	0.40	49 (8%) 10 10	57, 127, 181, 210	0
2	B	412/444 (92%)	0.03	10 (2%) 59 56	59, 103, 142, 171	0
2	D	412/444 (92%)	0.17	19 (4%) 32 30	66, 118, 161, 179	0
3	E	33/38 (86%)	-0.53	0 100 100	93, 131, 145, 166	0
3	F	33/38 (86%)	-0.55	0 100 100	110, 143, 170, 178	0
All	All	1998/2074 (96%)	0.23	120 (6%) 21 21	56, 115, 172, 210	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	LEU	8.5
1	C	133	PRO	7.6
1	C	29	GLU	6.8
1	A	135	ILE	6.0
1	A	136	ASN	5.9
1	C	252	TRP	5.8
1	C	293	ILE	5.7
1	A	554	ALA	5.6
1	C	135	ILE	5.5
1	A	71	TRP	5.5
1	C	33	ALA	5.5
1	C	25	PRO	5.4
1	A	67	ASP	5.3
1	C	138	GLU	5.1
1	C	30	LYS	5.1
1	A	133	PRO	5.0
1	C	134	SER	4.9
2	B	4	PRO	4.9
2	D	214	LEU	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	4.9
1	C	260	LEU	4.8
1	A	131	THR	4.7
1	C	257	ILE	4.6
1	C	32	LYS	4.6
2	B	5	ILE	4.6
1	C	27	THR	4.5
1	A	134	SER	4.5
1	C	28	GLU	4.5
1	C	289	LEU	4.4
1	A	549	ASP	4.4
1	A	26	LEU	4.3
1	C	60	VAL	4.3
1	C	132	ILE	4.3
1	C	61	PHE	4.2
1	A	553	SER	4.2
1	C	136	ASN	4.1
2	B	215	THR	4.1
1	A	73	LYS	4.0
1	C	74	LEU	4.0
1	A	550	LYS	3.8
1	A	148	VAL	3.8
1	C	142	ILE	3.8
1	C	130	PHE	3.8
2	B	92	LEU	3.6
1	A	545	ASN	3.5
2	D	215	THR	3.4
1	C	137	ASN	3.3
1	A	282	LEU	3.3
1	A	30	LYS	3.3
1	C	294	PRO	3.2
2	D	182	GLN	3.2
2	D	209	LEU	3.1
1	A	60	VAL	3.1
1	C	141	GLY	3.1
2	B	90	VAL	3.1
1	A	548	VAL	3.1
1	A	544	GLY	3.0
1	A	140	PRO	3.0
1	C	75	VAL	2.9
2	D	212	TRP	2.9
2	D	232	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	146	TYR	2.9
1	A	252	TRP	2.9
1	C	131	THR	2.9
1	C	139	THR	2.9
1	A	68	SER	2.9
2	D	422	LEU	2.9
1	C	277	ARG	2.9
2	B	252	TRP	2.9
1	A	251	SER	2.8
1	A	294	PRO	2.8
1	A	124	PHE	2.8
1	A	293	ILE	2.8
1	A	260	LEU	2.8
2	D	213	GLY	2.8
1	C	292	VAL	2.8
2	D	4	PRO	2.7
2	D	324	ASP	2.7
2	D	174	GLN	2.7
1	C	205	LEU	2.7
1	C	247	PRO	2.7
2	D	325	LEU	2.7
1	A	299	ALA	2.7
1	A	66	LYS	2.6
1	C	279	LEU	2.6
1	A	132	ILE	2.6
2	B	87	PHE	2.5
1	C	275	LYS	2.5
2	B	88	TRP	2.5
1	C	554	ALA	2.5
1	A	141	GLY	2.5
2	B	295	LEU	2.4
1	A	546	GLU	2.4
2	D	231	GLY	2.4
1	C	280	SER	2.4
1	A	137	ASN	2.3
1	C	64	LYS	2.3
1	A	283	LEU	2.3
1	C	73	LYS	2.3
1	A	142	ILE	2.3
1	A	62	ALA	2.3
1	C	281	LYS	2.2
1	A	74	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	GLU	2.2
1	C	299	ALA	2.2
1	C	144	TYR	2.2
2	D	171	PHE	2.2
1	C	288	ALA	2.2
1	A	70	LYS	2.2
2	D	73	LYS	2.2
2	D	211	ARG	2.2
1	C	297	GLU	2.2
2	D	92	LEU	2.1
1	C	17	ASP	2.1
1	C	181	TYR	2.1
2	D	89	GLU	2.1
1	C	256	ASP	2.1
1	A	542	ILE	2.0
1	C	276	VAL	2.0
2	D	210	LEU	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, 95^{th} 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	OMC	E	3	21/22	0.93	0.19	102,118,122,127	0
3	OMC	E	5	21/22	0.93	0.25	84,98,104,109	0
3	OMC	F	5	21/22	0.93	0.28	113,123,128,130	0
3	OMC	F	3	21/22	0.96	0.24	117,124,130,144	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

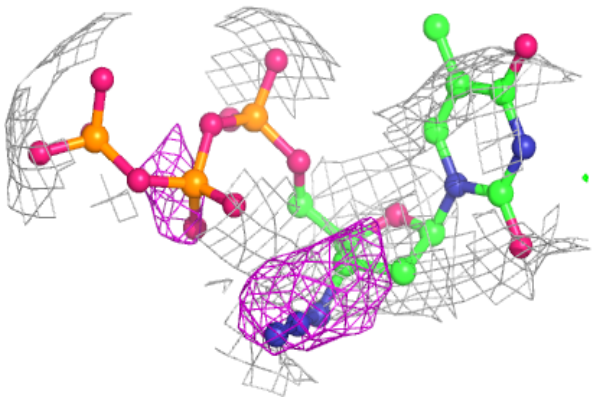
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

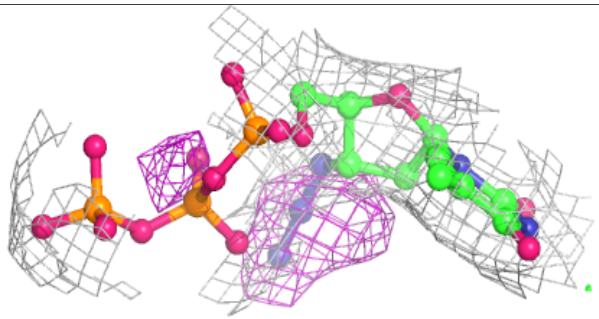
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	AZT	A	602	31/31	0.92	0.18	128,142,157,160	0
4	CA	C	601	1/1	0.94	0.11	170,170,170,170	0
4	CA	A	601	1/1	0.94	0.09	150,150,150,150	0
5	AZT	C	602	31/31	0.94	0.18	134,150,161,167	0

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 AZT A 602:

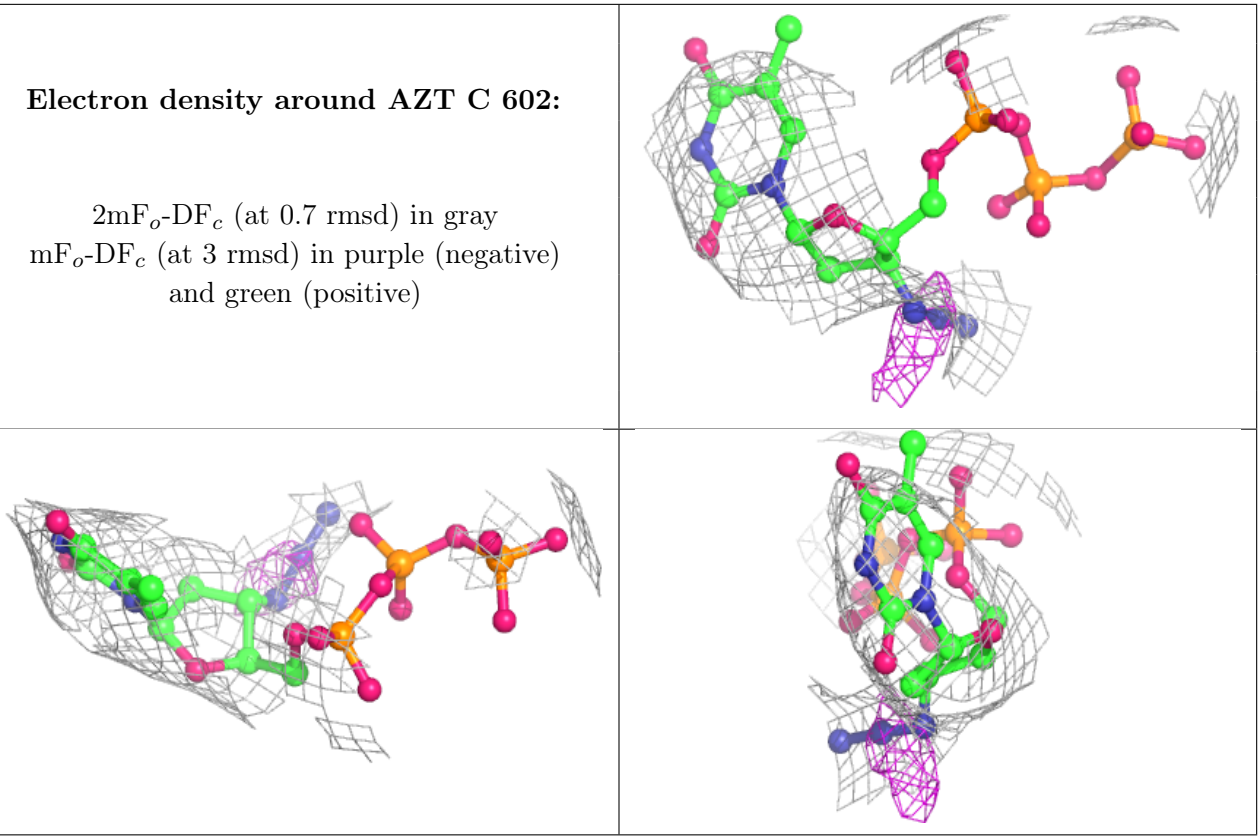
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around AZT C 602:

$2mF_o$-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 (i)

There are no such residues in this entry.