



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2016 – 07:19 PM EDT

PDB ID : 5HP1  
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX  
WITH A DNA aptamer and FOSCARNET, a Pyrophosphate analog  
Authors : Das, K.; Arnold, E.  
Deposited on : 2016-01-19  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

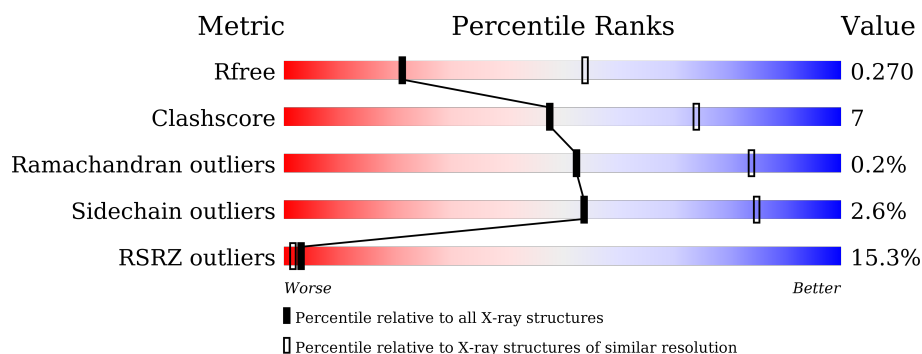
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	555	<div> <div>16%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	C	555	<div> <div>25%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
2	B	444	<div> <div>7%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
2	D	444	<div> <div>9%</div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
3	E	38	<div> <div>68%</div> <div>24%</div> <div>8%</div> </div>
3	F	38	<div> <div>63%</div> <div>29%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	B	2002	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17386 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	553	Total	C	N	O	S	0	0	0
			4494	2909	747	831	7			
1	C	553	Total	C	N	O	S	0	0	0
			4495	2910	748	830	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	416	Total	C	N	O	S	0	0	0
			3430	2234	567	622	7			
2	D	410	Total	C	N	O	S	0	1	0
			3391	2212	559	614	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

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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

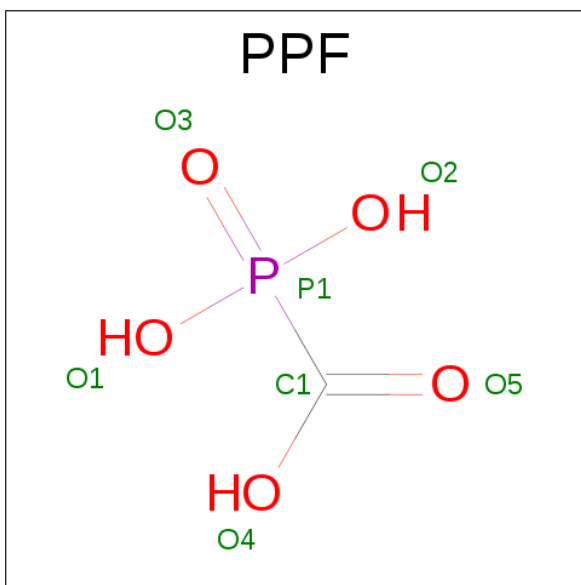
- Molecule 3 is a DNA chain called DNA (38-MER).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

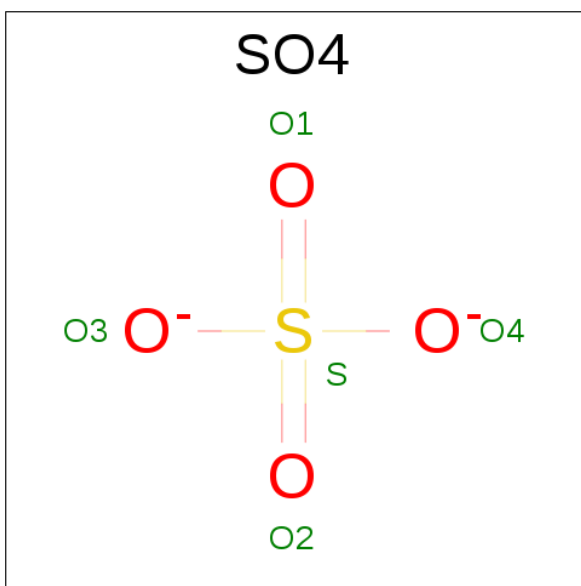
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Mg	0	0
			4	4		
4	C	4	Total	Mg	0	0
			4	4		

- Molecule 5 is PHOSPHONOFORMIC ACID (three-letter code: PPF) (formula: CH<sub>3</sub>O<sub>5</sub>P).



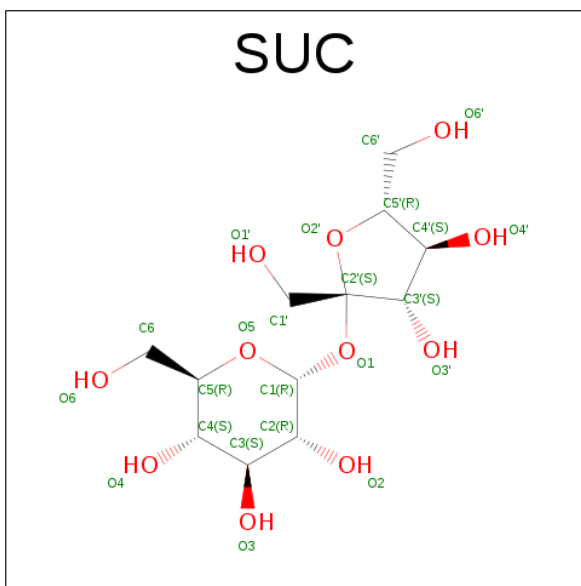
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			7	1	5	1		
5	C	1	Total	C	O	P	0	0
			7	1	5	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



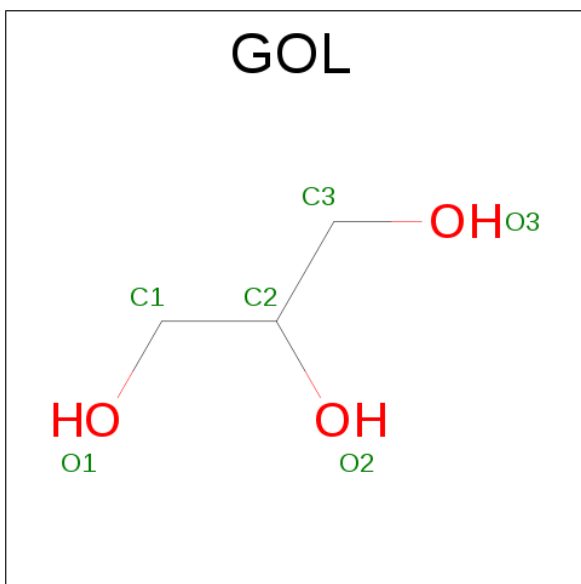
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is SUCROSE (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			23	12	11		
7	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



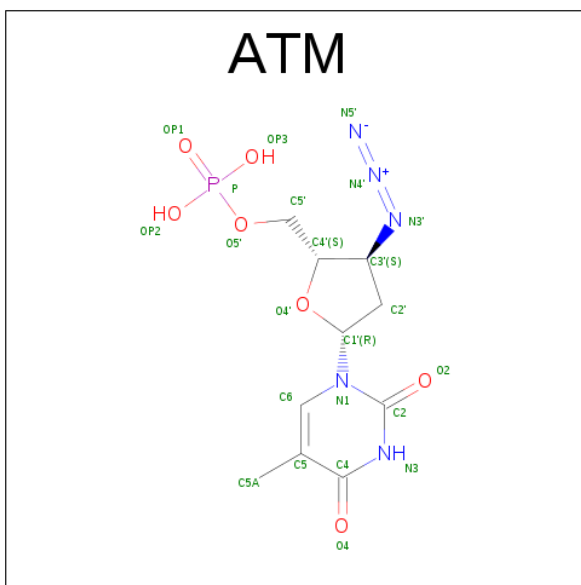
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 3'-AZIDO-3'-DEOXYTHYMIDINE-5'-MONOPHOSPHATE (three-letter code: ATM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	F	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
9	E	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 10 is water.

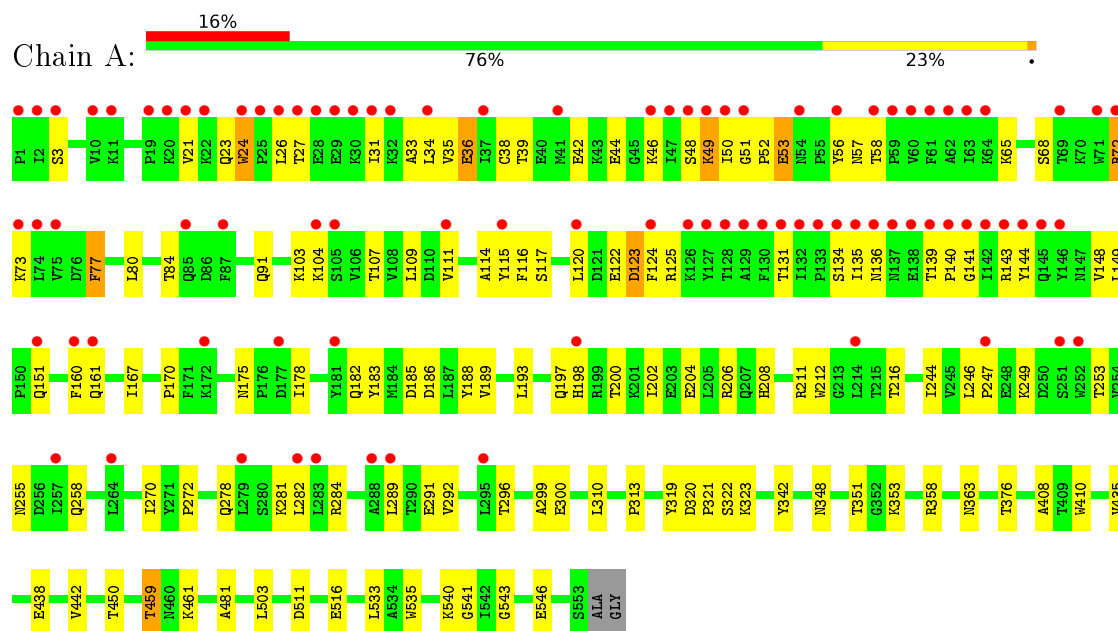
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	C	1	Total	O	0	0
			1	1		



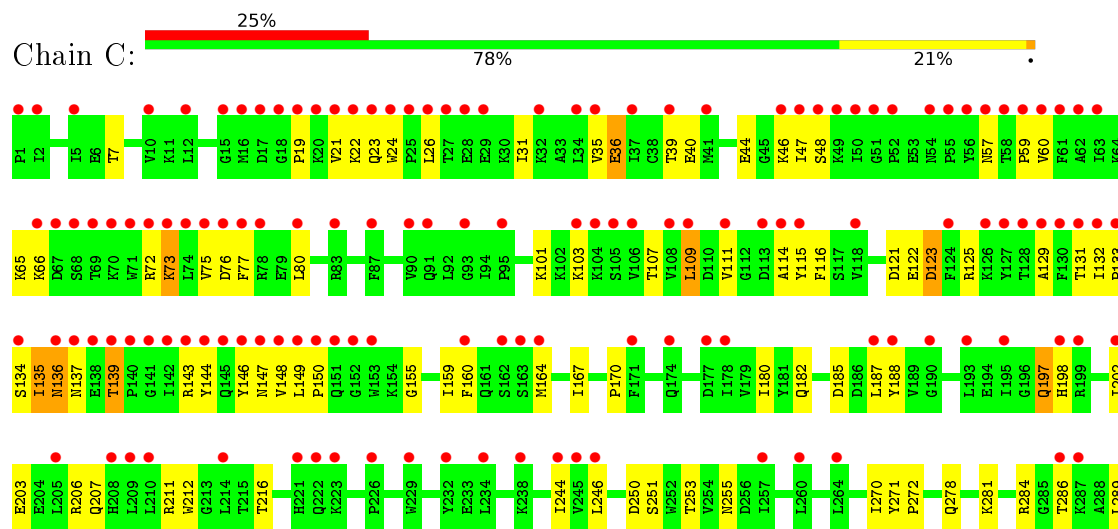
### 3 Residue-property plots

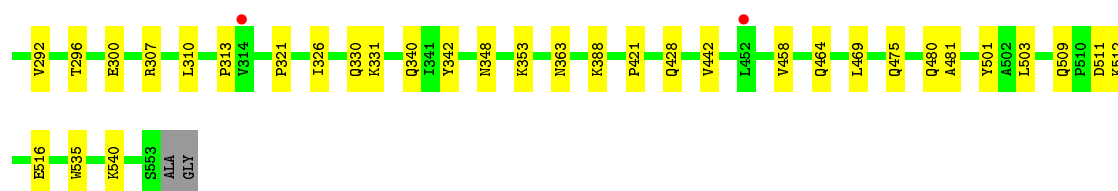
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

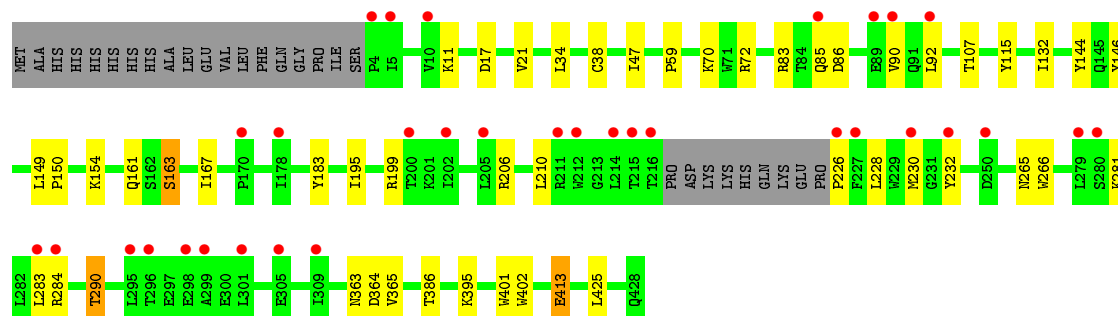
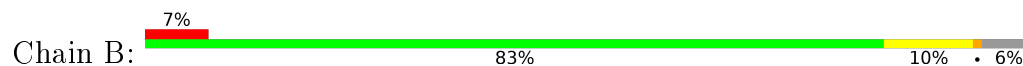


#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

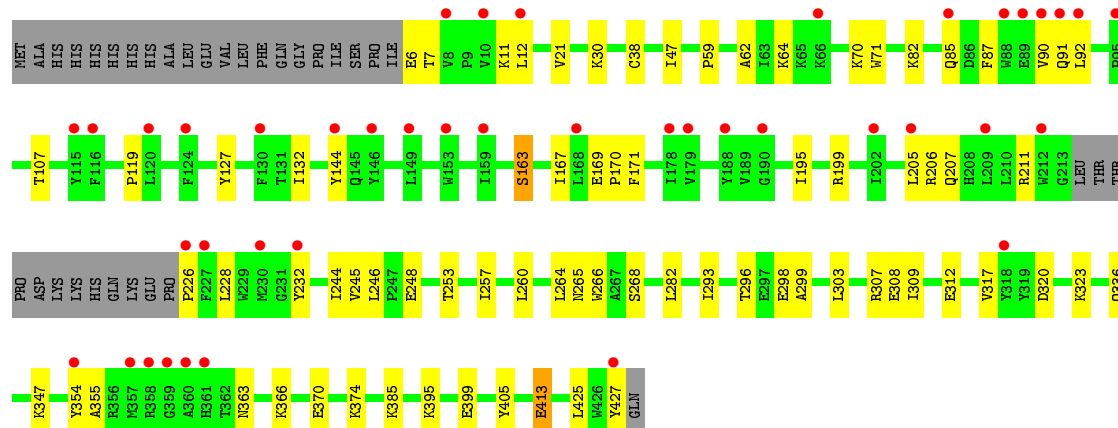
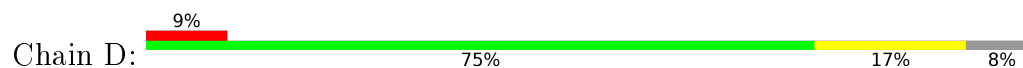




• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



• Molecule 3: DNA (38-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.33Å 129.07Å 131.54Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.90 45.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.64-2.90) 96.5 (45.64-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.246 , 0.273 0.246 , 0.270	Depositor DCC
$R_{free}$ test set	2552 reflections (4.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GOL, MG, SUC, PPF, ATM, 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	0.28	0/4612	0.50	0/6268
1	C	0.27	0/4613	0.54	1/6268 (0.0%)
2	B	0.28	0/3528	0.49	0/4791
2	D	0.29	0/3493	0.55	2/4747 (0.0%)
3	E	0.58	0/759	1.03	3/1170 (0.3%)
3	F	0.58	0/759	1.03	3/1170 (0.3%)
All	All	0.31	0/17764	0.59	9/24414 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	0	DA	O4'-C4'-C3'	-6.29	101.98	104.50
2	D	245	VAL	C-N-CA	-6.16	106.31	121.70
3	E	33	DG	O4'-C4'-C3'	-6.09	102.06	104.50
2	D	308	GLU	CA-CB-CG	5.96	126.50	113.40
3	F	31	DG	C4'-C3'-C2'	-5.54	98.11	103.10
3	E	31	DG	C4'-C3'-C2'	-5.40	98.24	103.10
1	C	139	THR	C-N-CD	-5.39	108.73	120.60
3	F	31	DG	O4'-C4'-C3'	-5.26	102.40	104.50
3	F	33	DG	O4'-C4'-C3'	-5.25	102.40	104.50

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	4494	0	4538	90	0
1	C	4495	0	4549	78	1
2	B	3430	0	3460	37	0
2	D	3391	0	3411	48	1
3	E	720	0	396	6	0
3	F	720	0	396	8	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	7	0	0	1	0
5	C	7	0	0	1	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	B	23	0	22	3	0
7	D	23	0	22	1	0
8	B	12	0	16	2	0
9	E	22	0	12	1	0
9	F	22	0	12	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
All	All	17386	0	16834	253	1

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 7.

All (253) 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:206:ARG:NH2	2:B:230:MET:O	2.02	0.94
2:B:70:LYS:HG3	2:B:226:PRO:HD2	1.53	0.90
1:C:134:SER:HG	1:C:139:THR:HG1	1.14	0.86
1:C:122:GLU:HA	1:C:125:ARG:HE	1.41	0.83
1:C:330:GLN:HE22	1:C:340:GLN:HE22	1.24	0.83
1:A:134:SER:OG	1:A:139:THR:OG1	1.96	0.81
1:A:56:TYR:O	1:A:143:ARG:NH1	2.15	0.77
1:A:91:GLN:OE1	1:A:161:GLN:NE2	2.17	0.77
1:C:23:GLN:HG2	1:C:133:PRO:HD3	1.65	0.76
1:C:22:LYS:O	1:C:59:PRO:HG3	1.86	0.76
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.69	0.75
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LYS:H	1:C:73:LYS:HD3	1.53	0.73
2:B:402:TRP:HE1	8:B:2003:GOL:H32	1.54	0.72
2:D:320:ASP:HB3	2:D:323:LYS:HE2	1.72	0.72
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.71	0.70
3:F:18:DT:H4'	3:F:19:DG:C8	2.29	0.68
2:D:206:ARG:HG3	2:D:228:LEU:HG	1.76	0.68
1:A:459:THR:HG22	1:A:461:LYS:H	1.59	0.67
2:D:85:GLN:HE21	2:D:90:VAL:HG21	1.60	0.66
1:A:73:LYS:O	1:A:151:GLN:NE2	2.29	0.66
1:C:26:LEU:HD22	1:C:132:ILE:HG13	1.79	0.64
1:A:65:LYS:HB2	1:A:68:SER:HB3	1.80	0.64
1:A:65:LYS:HE2	1:A:72:ARG:NH1	2.13	0.64
1:C:206:ARG:NH2	1:C:216:THR:O	2.30	0.63
1:A:122:GLU:HA	1:A:125:ARG:HE	1.62	0.63
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.81	0.62
1:C:123:ASP:OD1	1:C:123:ASP:N	2.33	0.61
2:B:206:ARG:NH2	2:B:228:LEU:O	2.29	0.61
1:C:21:VAL:O	1:C:57:ASN:ND2	2.34	0.61
2:D:266:TRP:CE3	2:D:425:LEU:HD22	2.35	0.61
1:A:206:ARG:NH2	1:A:216:THR:O	2.34	0.60
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.83	0.60
1:A:123:ASP:N	1:A:123:ASP:OD1	2.34	0.60
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.37	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.03	0.59
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.84	0.59
1:C:65:LYS:HB2	1:C:72:ARG:HG3	1.85	0.59
2:D:195:ILE:HD11	2:D:199:ARG:HE	1.67	0.59
1:A:410:TRP:CD1	2:B:363:ASN:HA	2.39	0.58
1:C:278:GLN:OE1	1:C:281:LYS:NZ	2.36	0.58
1:C:40:GLU:O	1:C:44:GLU:HG2	2.04	0.57
2:D:70:LYS:HG3	2:D:226:PRO:HD2	1.86	0.57
1:A:52:PRO:HG2	1:A:53:GLU:HG2	1.85	0.57
1:A:178:ILE:HD11	1:A:189:VAL:HG13	1.87	0.57
1:A:3:SER:HB2	1:A:211:ARG:HH22	1.71	0.56
1:C:203:GLU:O	1:C:207:GLN:HG2	2.05	0.56
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.45	0.56
2:D:246:LEU:HD13	2:D:260:LEU:HD11	1.88	0.56
1:C:47:ILE:HG22	1:C:146:TYR:HA	1.87	0.56
2:D:363:ASN:ND2	2:D:405:TYR:OH	2.39	0.56
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.06	0.55
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:O	2:B:161:GLN:NE2	2.39	0.55
1:C:331:LYS:HD3	1:C:421:PRO:HG2	1.89	0.55
1:A:175:ASN:O	1:A:178:ILE:HG22	2.07	0.55
1:A:49:LYS:H	1:A:49:LYS:HD3	1.72	0.54
1:C:65:LYS:HE3	1:C:72:ARG:NH2	2.22	0.54
1:A:459:THR:CG2	1:A:461:LYS:H	2.21	0.54
2:B:281:LYS:O	2:B:284:ARG:HG3	2.07	0.54
2:D:207:GLN:O	2:D:211:ARG:HG3	2.08	0.54
1:A:51:GLY:O	1:A:143:ARG:HD2	2.07	0.54
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.91	0.53
1:A:134:SER:HB3	1:A:141:GLY:HA2	1.90	0.53
7:B:2001:SUC:H6'1	7:B:2001:SUC:H62	1.90	0.53
1:A:278:GLN:OE1	1:A:281:LYS:NZ	2.41	0.53
1:C:73:LYS:H	1:C:73:LYS:CD	2.21	0.53
1:C:146:TYR:CG	1:C:150:PRO:HB3	2.44	0.53
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.91	0.52
2:D:6:GLU:OE1	2:D:6:GLU:N	2.42	0.52
1:C:65:LYS:HE3	1:C:72:ARG:HH21	1.75	0.52
2:D:395:LYS:HE2	2:D:399:GLU:OE2	2.10	0.52
1:C:115:TYR:CZ	9:E:101:ATM:H1'	2.45	0.52
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.45	0.52
2:D:296:THR:HG23	2:D:299:ALA:H	1.75	0.51
2:B:402:TRP:NE1	8:B:2003:GOL:H32	2.24	0.51
2:B:266:TRP:CE3	2:B:425:LEU:HD21	2.45	0.51
1:C:428:GLN:OE1	1:C:509:GLN:NE2	2.43	0.51
3:E:17:DT:H6	3:E:17:DT:C5'	2.24	0.51
3:E:18:DT:H4'	3:E:19:DG:C8	2.45	0.51
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.93	0.51
1:A:38:CYS:O	1:A:42:GLU:HG3	2.10	0.51
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.93	0.51
1:C:31:ILE:HG23	1:C:132:ILE:HD11	1.93	0.51
1:C:31:ILE:O	1:C:35:VAL:HG23	2.11	0.50
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.42	0.50
1:C:115:TYR:HB3	1:C:149:LEU:HB2	1.94	0.50
2:B:163:SER:O	2:B:167:ILE:HG13	2.11	0.50
2:D:309:ILE:O	2:D:312:GLU:HG2	2.12	0.50
1:A:51:GLY:H	1:A:52:PRO:CD	2.25	0.49
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.94	0.49
2:D:87:PHE:HB3	2:D:92:LEU:HB2	1.94	0.49
1:C:65:LYS:NZ	5:C:601:PPF:O5	2.28	0.49
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ALA:HA	1:C:144:TYR:O	2.11	0.49
2:D:244:ILE:HD11	2:D:425:LEU:HD21	1.94	0.49
1:A:3:SER:CB	1:A:211:ARG:HH12	2.26	0.49
1:A:200:THR:O	1:A:204:GLU:HG3	2.13	0.49
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.48	0.49
1:A:3:SER:HB2	1:A:211:ARG:NH2	2.28	0.48
1:A:23:GLN:HE21	1:A:26:LEU:HD11	1.78	0.48
1:C:469:LEU:HD11	1:C:480:GLN:HG2	1.95	0.48
2:D:253:THR:O	2:D:257:ILE:HD12	2.12	0.48
1:A:42:GLU:OE2	1:A:144:TYR:OH	2.25	0.48
1:C:65:LYS:HG3	1:C:72:ARG:HE	1.77	0.48
2:D:11:LYS:O	2:D:85:GLN:HB3	2.13	0.48
1:A:167:ILE:O	1:A:170:PRO:HD2	2.14	0.48
1:A:281:LYS:O	1:A:284:ARG:HG2	2.13	0.48
2:D:257:ILE:HD13	2:D:293:ILE:HD11	1.95	0.48
2:B:266:TRP:CZ3	2:B:425:LEU:HD21	2.48	0.48
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.95	0.48
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.95	0.48
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.14	0.48
1:C:458:VAL:HG23	1:C:464:GLN:HG2	1.96	0.48
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.13	0.47
1:C:540:LYS:HE3	2:D:265:ASN:OD1	2.14	0.47
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47
1:A:24:TRP:CZ2	3:F:-1:DT:H2'	2.50	0.47
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.95	0.47
2:B:17:ASP:O	2:B:83:ARG:HD3	2.13	0.47
1:C:73:LYS:N	1:C:73:LYS:HD3	2.24	0.47
1:C:353:LYS:NZ	3:E:7:DC:OP1	2.47	0.47
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.35	0.47
1:C:101:LYS:HE2	1:C:321:PRO:HG3	1.97	0.47
2:D:296:THR:CG2	2:D:299:ALA:H	2.28	0.47
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.50	0.47
2:B:11:LYS:O	2:B:85:GLN:HB3	2.14	0.47
2:D:303:LEU:O	2:D:307:ARG:HG3	2.15	0.47
1:A:120:LEU:H	1:A:148:VAL:HA	1.79	0.47
1:C:253:THR:HA	1:C:292:VAL:HA	1.97	0.47
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.48	0.47
1:C:76:ASP:OD2	3:E:-1:DT:H2''	2.14	0.47
1:A:21:VAL:O	1:A:57:ASN:ND2	2.47	0.46
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.97	0.46
2:B:85:GLN:HE21	2:B:90:VAL:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.42	0.46
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.98	0.46
2:D:12:LEU:HD11	2:D:127:TYR:CZ	2.51	0.46
2:B:413:GLU:HG3	7:B:2001:SUC:O6	2.15	0.46
2:B:72:ARG:HG2	2:B:226:PRO:HB3	1.98	0.46
1:A:198:HIS:O	1:A:202:ILE:HG12	2.16	0.46
1:A:296:THR:O	1:A:300:GLU:HG2	2.16	0.46
2:D:30:LYS:NZ	2:D:62:ALA:O	2.47	0.46
1:A:540:LYS:HE3	2:B:265:ASN:OD1	2.16	0.45
1:C:109:LEU:HD12	1:C:187:LEU:HB2	1.98	0.45
2:D:163:SER:O	2:D:167:ILE:HG13	2.15	0.45
3:F:4:OMC:H1'	3:F:4:OMC:HM23	1.74	0.45
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.97	0.45
1:A:182:GLN:HG3	1:A:182:GLN:O	2.16	0.45
1:C:136:ASN:N	1:C:136:ASN:OD1	2.49	0.45
3:E:17:DT:H6	3:E:17:DT:H5'	1.81	0.45
1:A:46:LYS:HD2	1:A:116:PHE:O	2.16	0.45
1:A:202:ILE:O	1:A:206:ARG:HG3	2.17	0.45
1:C:255:ASN:ND2	1:C:289:LEU:HD13	2.31	0.45
1:C:131:THR:HG22	1:C:143:ARG:CG	2.47	0.45
1:C:326:ILE:HD13	1:C:388:LYS:HB2	1.98	0.45
1:A:49:LYS:H	1:A:49:LYS:CD	2.30	0.45
2:D:366:LYS:O	2:D:370:GLU:HG3	2.16	0.45
1:A:320:ASP:OD1	1:A:322:SER:OG	2.20	0.45
1:C:180:ILE:HA	1:C:188:TYR:O	2.17	0.45
2:D:354:TYR:CE1	2:D:374:LYS:HD2	2.52	0.45
2:D:82:LYS:NZ	2:D:413:GLU:OE2	2.28	0.45
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.52	0.44
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.84	0.44
1:A:49:LYS:HA	1:A:144:TYR:CD1	2.53	0.44
1:A:543:GLY:N	2:B:283:LEU:O	2.49	0.44
1:C:511:ASP:OD1	1:C:512:LYS:NZ	2.48	0.44
1:A:115:TYR:HB3	1:A:149:LEU:O	2.18	0.44
1:A:255:ASN:HD22	1:A:289:LEU:HD13	1.81	0.44
1:A:58:THR:HG21	1:A:77:PHE:CE1	2.52	0.44
3:F:23:DC:H2''	3:F:24:DG:C8	2.52	0.44
2:B:115:TYR:O	2:B:149:LEU:HB2	2.18	0.44
1:C:36:GLU:O	1:C:40:GLU:HG2	2.18	0.44
1:A:435:VAL:HG13	2:B:290:THR:HG21	2.00	0.43
1:C:133:PRO:HB3	1:C:137:ASN:H	1.82	0.43
1:A:24:TRP:CH2	3:F:-1:DT:H2'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:ASP:CB	2:D:323:LYS:HE2	2.46	0.43
2:D:336:GLN:OE1	2:D:355:ALA:HB2	2.19	0.43
2:B:183:TYR:OH	2:B:386:THR:HG23	2.18	0.43
1:A:353:LYS:NZ	3:F:7:DC:OP1	2.51	0.43
1:C:296:THR:O	1:C:300:GLU:HG2	2.19	0.43
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.46	0.43
2:D:323:LYS:O	2:D:385:LYS:NZ	2.51	0.43
1:C:198:HIS:O	1:C:202:ILE:HG12	2.18	0.43
1:A:27:THR:O	1:A:31:ILE:HG13	2.18	0.43
1:A:50:ILE:HG23	1:A:52:PRO:HD2	2.01	0.43
1:A:51:GLY:N	1:A:52:PRO:CD	2.82	0.43
1:A:26:LEU:O	1:A:31:ILE:HD11	2.18	0.43
1:A:503:LEU:HA	1:A:503:LEU:HD12	1.70	0.43
1:A:26:LEU:HD23	1:A:34:LEU:CD1	2.49	0.42
1:C:19:PRO:HG3	1:C:80:LEU:HB2	2.02	0.42
1:C:182:GLN:HG3	1:C:182:GLN:O	2.18	0.42
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.86	0.42
2:D:298:GLU:OE1	2:D:298:GLU:N	2.45	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.19	0.42
1:A:51:GLY:HA3	1:A:143:ARG:HB2	2.01	0.42
2:B:395:LYS:NZ	7:B:2001:SUC:O4'	2.50	0.42
2:D:413:GLU:HG3	7:D:501:SUC:O6	2.19	0.42
2:D:70:LYS:HE2	2:D:70:LYS:HB2	1.77	0.42
1:A:33:ALA:O	1:A:36:GLU:HG3	2.19	0.42
2:B:210:LEU:O	2:B:210:LEU:HD12	2.19	0.42
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.50	0.41
1:A:253:THR:HA	1:A:292:VAL:HA	2.01	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.56	0.41
1:C:164:MET:HE2	1:C:187:LEU:HD21	2.02	0.41
1:C:167:ILE:O	1:C:170:PRO:HD2	2.20	0.41
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.51	0.41
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.54	0.41
1:A:183:TYR:OH	3:F:32:DG:N3	2.41	0.41
1:A:282:LEU:HD11	1:A:299:ALA:HB1	2.02	0.41
1:C:211:ARG:HG2	1:C:212:TRP:CD1	2.55	0.41
2:B:266:TRP:CE3	2:B:425:LEU:HD11	2.56	0.41
1:C:197:GLN:HG3	1:C:197:GLN:H	1.71	0.41
1:C:342:TYR:HB3	1:C:348:ASN:HA	2.02	0.41
2:D:169:GLU:HB3	2:D:170:PRO:HD3	2.02	0.41
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASP:O	1:C:125:ARG:HG3	2.20	0.41
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.20	0.41
1:C:270:ILE:O	1:C:272:PRO:HD3	2.21	0.41
1:C:300:GLU:HG2	1:C:300:GLU:H	1.65	0.41
1:A:503:LEU:HD11	1:A:533:LEU:HB3	2.03	0.41
2:B:107:THR:HA	2:B:232:TYR:O	2.20	0.41
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.03	0.41
1:C:103:LYS:HD3	1:C:103:LYS:HA	1.82	0.41
1:C:46:LYS:O	1:C:147:ASN:HB2	2.20	0.41
1:A:80:LEU:HD11	1:A:124:PHE:CZ	2.55	0.41
1:A:72:ARG:NH2	5:A:602:PPF:O1	2.49	0.41
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.56	0.41
1:C:271:TYR:CD2	1:C:310:LEU:HD23	2.55	0.41
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.55	0.41
2:D:265:ASN:O	2:D:268:SER:OG	2.34	0.41
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.56	0.41
2:B:11:LYS:HB3	2:B:11:LYS:HE3	1.80	0.41
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.55	0.41
2:D:317:VAL:HG12	2:D:347:LYS:HB3	2.03	0.41
1:A:208:HIS:O	1:A:212:TRP:HD1	2.04	0.40
1:A:258:GLN:OE1	3:F:28:DG:H2"	2.21	0.40
1:A:342:TYR:HB3	1:A:348:ASN:HA	2.02	0.40
2:B:72:ARG:HB2	2:B:226:PRO:HD3	2.02	0.40
1:C:155:GLY:O	1:C:159:ILE:HG12	2.21	0.40
1:C:503:LEU:HD12	1:C:503:LEU:HA	1.76	0.40
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.40
1:A:104:LYS:HD2	1:A:193:LEU:O	2.21	0.40
2:D:260:LEU:HD21	2:D:303:LEU:HD21	2.03	0.40
1:C:44:GLU:HB2	1:C:46:LYS:HD2	2.02	0.40
2:D:282:LEU:HD21	2:D:296:THR:HG22	2.02	0.40
1:C:246:LEU:HD13	1:C:307:ARG:HD3	2.04	0.40
1:C:284:ARG:HG2	3:E:8:DT:H5"	2.03	0.40
1:A:80:LEU:O	1:A:84:THR:OG1	2.31	0.40
1:C:116:PHE:HA	1:C:148:VAL:HG21	2.02	0.40
1:C:250:ASP:OD1	1:C:251:SER:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLN:NE2	2:D:91:GLN:OE1[2_657]	2.06	0.14

### 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	551/555 (99%)	526 (96%)	24 (4%)	1 (0%)	52	84
1	C	551/555 (99%)	526 (96%)	23 (4%)	2 (0%)	39	74
2	B	412/444 (93%)	399 (97%)	13 (3%)	0	100	100
2	D	407/444 (92%)	396 (97%)	11 (3%)	0	100	100
All	All	1921/1998 (96%)	1847 (96%)	71 (4%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	PRO
1	C	313	PRO
1	C	135	ILE

#### 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	492/495 (99%)	469 (95%)	23 (5%)	32	68
1	C	493/495 (100%)	477 (97%)	16 (3%)	46	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	376/403 (93%)	373 (99%)	3 (1%)	86	96
2	D	371/403 (92%)	368 (99%)	3 (1%)	86	96
All	All	1732/1796 (96%)	1687 (97%)	45 (3%)	54	85

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	36	GLU
1	A	39	THR
1	A	44	GLU
1	A	48	SER
1	A	49	LYS
1	A	53	GLU
1	A	72	ARG
1	A	77	PHE
1	A	109	LEU
1	A	117	SER
1	A	123	ASP
1	A	135	ILE
1	A	136	ASN
1	A	186	ASP
1	A	188	TYR
1	A	197	GLN
1	A	244	ILE
1	A	291	GLU
1	A	358	ARG
1	A	450	THR
1	A	459	THR
1	A	516	GLU
2	B	163	SER
2	B	290	THR
2	B	413	GLU
1	C	7	THR
1	C	24	TRP
1	C	36	GLU
1	C	39	THR
1	C	48	SER
1	C	66	LYS
1	C	73	LYS
1	C	77	PHE

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Mol	Chain	Res	Type
1	C	109	LEU
1	C	123	ASP
1	C	135	ILE
1	C	136	ASN
1	C	197	GLN
1	C	244	ILE
1	C	286	THR
1	C	516	GLU
2	D	163	SER
2	D	413	GLU
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	ASN
1	C	151	GLN
1	C	340	GLN
1	C	428	GLN
1	C	509	GLN
1	C	545	ASN

### 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	E	2	3	15,22,23	3.12	6 (40%)	20,31,34	1.55	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMC	E	4	3	15,22,23	3.05	6 (40%)	20,31,34	1.61	1 (5%)
3	OMC	F	2	3	15,22,23	3.08	6 (40%)	20,31,34	1.63	1 (5%)
3	OMC	F	4	3	15,22,23	3.10	6 (40%)	20,31,34	1.68	1 (5%)

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	E	2	3	-	0/5/27/28	0/2/2/2
3	OMC	E	4	3	-	0/5/27/28	0/2/2/2
3	OMC	F	2	3	-	0/5/27/28	0/2/2/2
3	OMC	F	4	3	-	0/5/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C4-N4	2.30	1.41	1.35
3	E	2	OMC	C4-N4	2.31	1.41	1.35
3	F	4	OMC	C4-N4	2.32	1.41	1.35
3	F	2	OMC	C4-N4	2.35	1.41	1.35
3	E	4	OMC	C5-C4	2.56	1.47	1.41
3	F	2	OMC	C5-C4	2.58	1.47	1.41
3	E	2	OMC	C5-C4	2.59	1.47	1.41
3	F	4	OMC	C5-C4	2.62	1.47	1.41
3	E	4	OMC	C2-N3	4.57	1.47	1.38
3	F	2	OMC	C2-N3	4.68	1.47	1.38
3	E	2	OMC	C2-N3	4.69	1.47	1.38
3	F	4	OMC	C2-N3	4.71	1.48	1.38
3	E	4	OMC	C6-C5	4.91	1.48	1.38
3	E	2	OMC	C6-C5	4.93	1.48	1.38
3	F	2	OMC	C6-C5	4.94	1.48	1.38
3	F	4	OMC	C6-C5	5.01	1.49	1.38
3	F	2	OMC	C4-N3	5.24	1.45	1.35
3	E	4	OMC	C4-N3	5.26	1.45	1.35
3	F	4	OMC	C4-N3	5.28	1.45	1.35
3	E	2	OMC	C4-N3	5.31	1.45	1.35
3	E	4	OMC	C6-N1	7.38	1.45	1.35
3	F	2	OMC	C6-N1	7.44	1.45	1.35
3	F	4	OMC	C6-N1	7.48	1.45	1.35
3	E	2	OMC	C6-N1	7.65	1.45	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	OMC	C6-C5-C4	5.85	119.73	117.44
3	F	2	OMC	C6-C5-C4	6.36	119.93	117.44
3	E	4	OMC	C6-C5-C4	6.42	119.95	117.44
3	F	4	OMC	C6-C5-C4	6.79	120.10	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	OMC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	PPF	A	602	4	3,6,6	1.17	0	5,9,9	0.66	0
6	SO4	A	606	-	4,4,4	0.23	0	6,6,6	0.08	0
7	SUC	B	2001	-	24,24,24	0.42	0	36,36,36	0.64	0
8	GOL	B	2002	-	5,5,5	0.35	0	5,5,5	0.16	0
8	GOL	B	2003	-	5,5,5	0.38	0	5,5,5	0.30	0
5	PPF	C	601	4	3,6,6	1.06	0	5,9,9	0.79	0
6	SO4	C	605	-	4,4,4	0.21	0	6,6,6	0.06	0
7	SUC	D	501	-	24,24,24	0.43	0	36,36,36	0.66	0
9	ATM	E	101	3,4	13,23,24	1.35	1 (7%)	17,32,35	2.22	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	ATM	F	101	3,4	13,23,24	1.32	1 (7%)	17,32,35	2.36	4 (23%)

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	PPF	A	602	4	-	0/0/6/6	0/0/0/0
6	SO4	A	606	-	-	0/0/0/0	0/0/0/0
7	SUC	B	2001	-	-	0/12/51/51	0/2/2/2
8	GOL	B	2002	-	-	0/4/4/4	0/0/0/0
8	GOL	B	2003	-	-	0/4/4/4	0/0/0/0
5	PPF	C	601	4	-	0/0/6/6	0/0/0/0
6	SO4	C	605	-	-	0/0/0/0	0/0/0/0
7	SUC	D	501	-	-	0/12/51/51	0/2/2/2
9	ATM	E	101	3,4	-	0/6/24/25	0/2/2/2
9	ATM	F	101	3,4	-	0/6/24/25	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	ATM	C4-N3	3.99	1.40	1.33
9	E	101	ATM	C4-N3	4.32	1.40	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	ATM	C5-C4-N3	-6.12	120.21	125.35
9	E	101	ATM	C5-C4-N3	-6.07	120.25	125.35
9	E	101	ATM	C2'-C1'-N1	-2.47	108.06	114.14
9	F	101	ATM	C3'-N3'-N4'	2.11	121.86	115.83
9	F	101	ATM	O4'-C1'-N1	3.25	113.40	107.71
9	F	101	ATM	C4-N3-C2	5.32	119.60	115.16
9	E	101	ATM	C4-N3-C2	5.36	119.63	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	PPF	1	0
7	B	2001	SUC	3	0
8	B	2003	GOL	2	0
5	C	601	PPF	1	0
7	D	501	SUC	1	0
9	E	101	ATM	1	0

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	553/555 (99%)	0.87	90 (16%) <b>2</b> <b>1</b>	35, 103, 171, 223	0
1	C	553/555 (99%)	1.34	141 (25%) <b>1</b> <b>0</b>	35, 121, 215, 263	0
2	B	416/444 (93%)	0.49	33 (7%) <b>15</b> <b>10</b>	42, 82, 149, 195	0
2	D	410/444 (92%)	0.74	42 (10%) <b>9</b> <b>5</b>	37, 98, 167, 238	0
3	E	33/38 (86%)	0.37	0 <b>100</b> <b>100</b>	80, 118, 143, 210	0
3	F	33/38 (86%)	-0.07	0 <b>100</b> <b>100</b>	71, 103, 134, 175	0
All	All	1998/2074 (96%)	0.87	306 (15%) <b>3</b> <b>1</b>	35, 99, 191, 263	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	358	ARG	14.9
1	A	73	LYS	13.3
1	C	131	THR	11.2
1	C	26	LEU	11.0
1	A	71	TRP	9.8
1	C	24	TRP	9.3
1	C	137	ASN	9.3
1	C	52	PRO	9.1
1	C	58	THR	9.0
2	D	232	TYR	9.0
1	A	2	ILE	8.4
1	C	142	ILE	8.4
1	C	21	VAL	8.0
1	A	61	PHE	7.9
1	C	22	LYS	7.7
1	C	139	THR	7.6
1	A	3	SER	7.4
2	B	214	LEU	7.3
1	C	132	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
2	D	10	VAL	7.1
2	B	226	PRO	7.1
1	A	133	PRO	7.0
1	C	46	LYS	7.0
1	C	124	PHE	6.9
1	C	136	ASN	6.9
1	A	131	THR	6.8
2	D	90	VAL	6.8
1	A	62	ALA	6.8
1	A	72	ARG	6.8
1	C	50	ILE	6.8
2	B	299	ALA	6.7
1	A	46	LYS	6.7
1	C	145	GLN	6.6
1	C	75	VAL	6.5
1	C	111	VAL	6.4
1	C	55	PRO	6.4
1	C	1	PRO	6.3
1	C	2	ILE	6.3
1	C	25	PRO	6.2
1	C	133	PRO	6.2
1	C	146	TYR	6.1
1	A	134	SER	6.1
1	C	56	TYR	6.0
1	C	47	ILE	5.8
1	C	23	GLN	5.6
1	C	54	ASN	5.6
2	B	215	THR	5.5
1	C	138	GLU	5.5
1	C	49	LYS	5.5
1	A	75	VAL	5.5
1	A	143	ARG	5.5
1	C	34	LEU	5.5
1	C	130	PHE	5.5
1	A	59	PRO	5.4
1	C	61	PHE	5.4
2	D	226	PRO	5.4
1	C	205	LEU	5.3
1	A	60	VAL	5.3
1	C	35	VAL	5.2
1	A	26	LEU	5.1
1	C	193	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	229	TRP	5.1
1	A	142	ILE	5.0
1	C	141	GLY	4.9
1	C	174	GLN	4.9
1	A	74	LEU	4.9
1	C	114	ALA	4.9
1	A	21	VAL	4.8
1	A	128	THR	4.8
1	C	32	LYS	4.8
1	C	28	GLU	4.7
1	C	109	LEU	4.7
2	D	146	TYR	4.7
2	D	92	LEU	4.6
2	B	230	MET	4.6
2	D	227	PHE	4.6
1	C	134	SER	4.6
1	C	19	PRO	4.5
1	A	130	PHE	4.5
1	C	232	TYR	4.5
1	C	178	ILE	4.5
1	A	58	THR	4.5
1	A	144	TYR	4.4
1	C	76	ASP	4.4
2	B	216	THR	4.4
1	C	150	PRO	4.3
1	C	67	ASP	4.3
1	A	34	LEU	4.3
1	C	202	ILE	4.3
2	D	212	TRP	4.2
1	A	47	ILE	4.2
2	D	124	PHE	4.2
2	D	116	PHE	4.1
1	C	68	SER	4.1
1	A	49	LYS	4.1
2	D	202	ILE	4.1
1	C	127	TYR	4.1
1	C	80	LEU	4.1
1	A	135	ILE	4.0
2	B	296	THR	4.0
1	C	74	LEU	4.0
1	A	126	LYS	4.0
2	D	8	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	280	SER	3.9
2	D	230	MET	3.9
1	C	286	THR	3.9
1	C	103	LYS	3.9
1	A	124	PHE	3.9
1	C	60	VAL	3.9
1	A	146	TYR	3.8
1	C	73	LYS	3.8
1	A	50	ILE	3.8
1	C	108	VAL	3.8
2	B	90	VAL	3.8
2	B	250	ASP	3.8
1	C	187	LEU	3.8
1	C	148	VAL	3.8
1	C	48	SER	3.8
1	C	10	VAL	3.8
2	D	209	LEU	3.7
1	A	19	PRO	3.7
1	C	115	TYR	3.7
1	C	62	ALA	3.7
1	A	141	GLY	3.6
1	C	257	ILE	3.6
2	D	89	GLU	3.6
1	C	153	TRP	3.6
1	C	20	LYS	3.5
1	A	28	GLU	3.5
1	C	143	ARG	3.5
1	A	138	GLU	3.5
1	A	132	ILE	3.5
1	C	140	PRO	3.5
1	C	144	TYR	3.5
2	D	159	ILE	3.5
1	C	188	TYR	3.5
1	A	295	LEU	3.4
1	C	17	ASP	3.4
1	C	51	GLY	3.4
1	A	136	ASN	3.4
1	A	30	LYS	3.4
1	A	27	THR	3.4
1	A	1	PRO	3.4
1	A	140	PRO	3.3
1	C	59	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	115	TYR	3.3
1	A	137	ASN	3.3
1	C	221	HIS	3.3
2	D	168	LEU	3.3
1	A	24	TRP	3.3
1	C	39	THR	3.2
1	C	18	GLY	3.2
1	A	120	LEU	3.2
1	C	160	PHE	3.2
2	B	200	THR	3.2
1	A	151	GLN	3.2
2	B	89	GLU	3.2
1	A	25	PRO	3.2
1	A	139	THR	3.1
2	B	10	VAL	3.1
2	D	115	TYR	3.1
1	C	104	LYS	3.1
1	A	69	THR	3.1
1	A	54	ASN	3.1
1	C	41	MET	3.0
2	D	178	ILE	3.0
2	D	318	TYR	3.0
2	D	360	ALA	3.0
1	C	171	PHE	3.0
2	D	95	PRO	3.0
1	A	257	ILE	3.0
1	C	66	LYS	3.0
2	B	227	PHE	2.9
2	D	144	TYR	2.9
1	C	37	ILE	2.9
2	B	202	ILE	2.9
1	C	195	ILE	2.9
1	C	210	LEU	2.9
2	D	66	LYS	2.9
1	C	72	ARG	2.9
1	C	226	PRO	2.8
1	C	113	ASP	2.8
1	C	16	MET	2.8
2	B	92	LEU	2.8
2	D	88	TRP	2.8
1	C	93	GLY	2.8
1	C	199	ARG	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	129	ALA	2.8
2	B	85	GLN	2.8
1	A	145	GLN	2.8
2	B	283	LEU	2.8
2	B	295	LEU	2.8
1	C	29	GLU	2.7
2	B	298	GLU	2.7
1	C	177	ASP	2.7
1	C	57	ASN	2.7
1	A	177	ASP	2.7
1	C	287	LYS	2.7
1	A	10	VAL	2.7
2	B	211	ARG	2.7
1	A	31	ILE	2.7
1	A	22	LYS	2.7
1	A	172	LYS	2.7
2	D	359	GLY	2.7
1	A	283	LEU	2.7
1	A	51	GLY	2.7
1	C	198	HIS	2.7
2	D	427	TYR	2.7
1	C	260	LEU	2.6
2	D	85	GLN	2.6
1	A	251	SER	2.6
1	C	106	VAL	2.6
1	C	70	LYS	2.6
1	C	69	THR	2.6
1	C	5	ILE	2.6
1	C	223	LYS	2.6
1	C	208	HIS	2.6
2	D	361	HIS	2.6
1	A	37	ILE	2.6
1	C	214	LEU	2.5
2	D	190	GLY	2.5
1	C	83	ARG	2.5
1	C	238	LYS	2.5
1	A	279	LEU	2.5
1	A	63	ILE	2.5
2	D	357	MET	2.5
2	D	12	LEU	2.5
1	C	147	ASN	2.5
1	A	56	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLU	2.4
2	B	5	ILE	2.4
2	D	149	LEU	2.4
1	C	164	MET	2.4
1	C	63	ILE	2.4
1	C	234	LEU	2.4
1	A	20	LYS	2.4
1	A	64	LYS	2.4
1	C	246	LEU	2.4
1	C	264	LEU	2.4
1	A	87	PHE	2.4
1	A	282	LEU	2.4
1	C	128	THR	2.4
2	D	130	PHE	2.4
1	C	244	ILE	2.4
2	B	301	LEU	2.4
2	B	309	ILE	2.4
1	A	32	LYS	2.4
1	C	87	PHE	2.4
1	A	288	ALA	2.4
1	C	209	LEU	2.4
2	D	120	LEU	2.4
1	A	111	VAL	2.3
1	C	222	GLN	2.3
1	C	151	GLN	2.3
1	A	247	PRO	2.3
1	C	95	PRO	2.3
1	C	162	SER	2.3
2	D	179	VAL	2.3
1	C	27	THR	2.3
2	D	91	GLN	2.3
2	D	205	LEU	2.3
1	A	104	LYS	2.3
2	B	205	LEU	2.3
1	C	152	GLY	2.2
1	A	85	GLN	2.2
1	A	264	LEU	2.2
1	A	127	TYR	2.2
2	B	232	TYR	2.2
1	C	126	LYS	2.2
1	C	78	ARG	2.2
1	A	11	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	188	TYR	2.2
2	B	305	GLU	2.2
2	D	354	TYR	2.2
1	C	90	VAL	2.2
1	C	118	VAL	2.2
2	B	279	LEU	2.2
2	D	153	TRP	2.2
1	C	129	ALA	2.2
1	A	161	GLN	2.2
2	B	178	ILE	2.2
1	A	48	SER	2.1
2	B	170	PRO	2.1
1	A	160	PHE	2.1
2	B	4	PRO	2.1
1	A	214	LEU	2.1
1	C	452	LEU	2.1
1	C	15	GLY	2.1
1	C	12	LEU	2.1
1	C	77	PHE	2.1
1	A	181	TYR	2.1
1	C	105	SER	2.1
1	C	190	GLY	2.1
2	B	212	TRP	2.1
1	A	105	SER	2.0
1	C	163	SER	2.0
1	A	198	HIS	2.0
1	C	91	GLN	2.0
1	A	41	MET	2.0
1	C	245	VAL	2.0
2	B	284	ARG	2.0
1	A	289	LEU	2.0
1	C	149	LEU	2.0
1	A	252	TRP	2.0
1	C	71	TRP	2.0
1	C	314	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OMC	F	4	21/22	0.94	0.20	-	64,73,78,83	0
3	OMC	E	4	21/22	0.89	0.29	-	86,101,112,115	0
3	OMC	E	2	21/22	0.86	0.26	-	104,117,125,132	0
3	OMC	F	2	21/22	0.95	0.18	-	88,97,105,106	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GOL	B	2002	6/6	0.84	0.27	4.41	71,79,80,81	0
4	MG	C	602	1/1	0.64	0.17	1.03	62,62,62,62	0
8	GOL	B	2003	6/6	0.92	0.26	0.96	60,64,68,73	0
9	ATM	F	101	22/23	0.88	0.30	-0.21	141,148,164,171	0
4	MG	A	604	1/1	0.50	0.18	-0.33	130,130,130,130	0
7	SUC	D	501	23/23	0.90	0.20	-0.34	81,92,98,101	0
9	ATM	E	101	22/23	0.82	0.30	-0.57	121,134,156,168	0
5	PPF	A	602	7/7	0.72	0.20	-0.62	124,142,159,169	0
5	PPF	C	601	7/7	0.70	0.16	-1.33	150,162,172,189	0
4	MG	C	604	1/1	0.51	0.09	-1.50	166,166,166,166	0
4	MG	A	601	1/1	0.75	0.13	-2.06	80,80,80,80	0
7	SUC	B	2001	23/23	0.92	0.17	-2.56	64,81,90,94	0
6	SO4	C	605	5/5	0.90	0.11	-2.94	102,108,113,123	0
4	MG	A	605	1/1	0.87	0.16	-	80,80,80,80	0
4	MG	A	603	1/1	0.90	0.14	-	133,133,133,133	1
6	SO4	A	606	5/5	0.87	0.15	-	95,108,116,127	0
4	MG	C	603	1/1	0.92	0.11	-	156,156,156,156	0
4	MG	C	606	1/1	0.85	0.12	-	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.