



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:13 AM GMT

PDB ID : 4I2P  
Title : Crystal structure of HIV-1 reverse transcriptase in complex with rilpivirine (TMC278) based analogue  
Authors : Patel, D.; Bauman, J.D.; Das, K.; Arnold, E.  
Deposited on : 2012-11-22  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

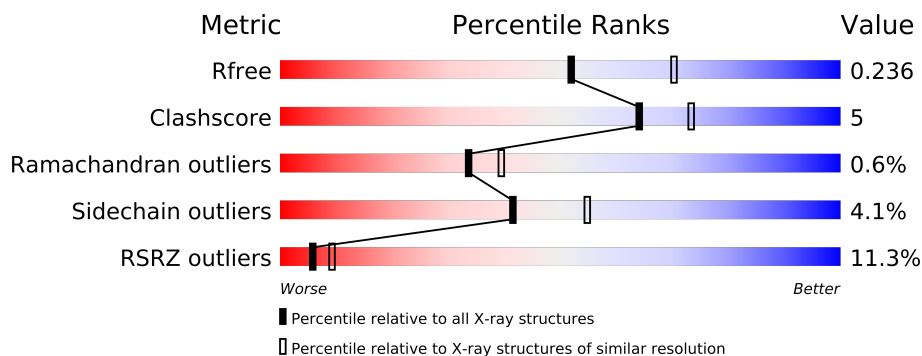
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	557	
2	B	428	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8249 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4505	2917	748	832	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	172	ALA	LYS	ENGINEERED MUTATION	UNP P03366
A	173	ALA	LYS	ENGINEERED MUTATION	UNP P03366
A	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

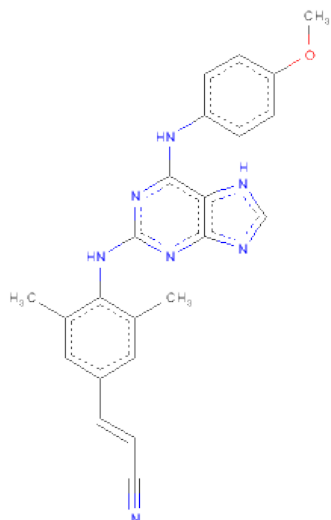
- Molecule 2 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3413	2225	564	617	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED MUTATION	UNP P03366

- Molecule 3 is (2E)-3-[4-({6-[(4-METHOXYPHENYL)AMINO]-7H-PURIN-2-YL}AMINO)-3,5-DIMETHYLPHENYL]PROP-2-ENENITRILE (three-letter code: G73) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>7</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	23	7	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	122	Total	O	0	0
			122	122		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.65Å 72.99Å 109.60Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	41.29 – 2.30 41.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (41.29-2.30) 98.8 (41.29-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.216 , 0.260 0.205 , 0.236	Depositor DCC
$R_{free}$ test set	894 reflections (1.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55926 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G73

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	0.27	0/4623	0.45	0/6284
2	B	0.26	0/3511	0.45	0/4768
All	All	0.27	0/8134	0.45	0/11052

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4505	0	4562	46	0
2	B	3413	0	3443	44	0
3	A	31	0	21	3	0
4	A	178	0	0	7	0
4	B	122	0	0	10	0
All	All	8249	0	8026	86	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:182:GLN:O	4:B:617:HOH:O	1.91	0.89
1:A:101:LYS:HE2	3:A:601:G73:H23	1.59	0.82
2:B:347:LYS:O	4:B:525:HOH:O	1.98	0.81
1:A:328:GLU:OE2	4:A:864:HOH:O	2.01	0.79
2:B:428:GLN:OXT	4:B:557:HOH:O	2.06	0.71
2:B:358:ARG:HH12	2:B:374:LYS:HD2	1.56	0.69
2:B:91:GLN:HG3	2:B:93:GLY:H	1.58	0.68
1:A:332:GLN:OE1	4:A:833:HOH:O	2.11	0.67
2:B:206:ARG:NH1	2:B:229:TRP:O	2.29	0.66
2:B:425:LEU:O	4:B:557:HOH:O	2.14	0.65
2:B:194:GLU:HB3	2:B:197:GLN:HG2	1.80	0.64
2:B:143:ARG:HD3	4:B:527:HOH:O	1.99	0.63
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.32	0.62
2:B:202:ILE:HG22	2:B:206:ARG:HE	1.64	0.62
1:A:216:THR:O	1:A:218:ASP:N	2.32	0.61
2:B:239:TRP:O	4:B:520:HOH:O	2.17	0.60
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.83	0.59
1:A:311:LYS:HE3	1:A:312:GLU:HG2	1.85	0.59
1:A:527:LYS:NZ	4:A:808:HOH:O	2.36	0.59
2:B:240:THR:O	2:B:350:LYS:NZ	2.31	0.58
1:A:257:ILE:HB	1:A:283:LEU:HD21	1.86	0.58
1:A:6:GLU:CD	1:A:6:GLU:H	2.07	0.57
1:A:360:ALA:HA	1:A:514:GLU:HG3	1.86	0.57
1:A:218:ASP:OD1	4:A:843:HOH:O	2.18	0.56
1:A:206:ARG:HE	1:A:216:THR:HG1	1.54	0.55
3:A:601:G73:N11	3:A:601:G73:H5	2.22	0.55
1:A:206:ARG:CZ	1:A:218:ASP:HB2	2.37	0.54
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.43	0.54
1:A:101:LYS:H	3:A:601:G73:H22	1.55	0.54
1:A:88:TRP:NE1	2:B:143:ARG:HD2	2.22	0.54
2:B:425:LEU:HD13	2:B:428:GLN:HB3	1.90	0.54
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.91	0.53
2:B:161:GLN:O	2:B:165:THR:OG1	2.26	0.53
2:B:273:GLY:N	4:B:543:HOH:O	2.36	0.51
1:A:478:GLU:HG2	4:A:853:HOH:O	2.08	0.51
2:B:122:GLU:O	4:B:512:HOH:O	2.19	0.51
1:A:454:LYS:NZ	1:A:552:VAL:HB	2.26	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.50
2:B:198:HIS:O	2:B:202:ILE:HG12	2.11	0.50
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.93	0.50
1:A:28:GLU:HG2	1:A:32:LYS:HE3	1.93	0.50
1:A:491:LEU:HB3	1:A:529:GLU:HG2	1.95	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.12	0.49
2:B:70:LYS:O	4:B:536:HOH:O	2.20	0.49
2:B:208:HIS:O	2:B:212:TRP:HD1	1.95	0.49
1:A:258:GLN:HG2	1:A:283:LEU:HD13	1.93	0.49
1:A:543:GLY:N	2:B:283:LEU:O	2.46	0.48
1:A:317:VAL:HG23	1:A:349:LEU:HD12	1.94	0.48
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.94	0.48
2:B:239:TRP:N	4:B:520:HOH:O	2.46	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.95	0.48
1:A:544:GLY:O	1:A:546:GLU:N	2.48	0.47
1:A:369:THR:O	1:A:373:GLN:HG2	2.14	0.47
1:A:466:VAL:HG22	1:A:550:LYS:NZ	2.29	0.47
1:A:115:TYR:O	4:A:803:HOH:O	2.20	0.47
2:B:191:SER:HG	2:B:198:HIS:HD1	1.44	0.45
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.99	0.45
1:A:546:GLU:HA	4:A:750:HOH:O	2.17	0.45
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.99	0.45
2:B:191:SER:HG	2:B:198:HIS:CE1	2.35	0.44
1:A:547:GLN:O	1:A:551:LEU:N	2.47	0.44
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.99	0.44
1:A:466:VAL:HG22	1:A:550:LYS:HZ3	1.82	0.44
2:B:242:GLN:HB2	2:B:351:THR:OG1	2.17	0.44
1:A:196:GLY:HA2	1:A:199:ARG:HH21	1.83	0.44
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.44
1:A:68:SER:OG	1:A:69:THR:N	2.51	0.44
2:B:208:HIS:O	2:B:208:HIS:ND1	2.51	0.43
2:B:91:GLN:HB2	2:B:94:ILE:HG13	2.00	0.43
1:A:537:PRO:HB2	1:A:540:LYS:HG3	2.01	0.43
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
1:A:417:VAL:HG22	1:A:419:THR:HG23	2.01	0.43
1:A:281:LYS:HA	1:A:284:ARG:HG3	2.01	0.42
1:A:64:LYS:HD2	1:A:68:SER:O	2.19	0.42
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.55	0.42
2:B:315:HIS:O	2:B:347:LYS:NZ	2.42	0.42
2:B:277:ARG:HD3	2:B:277:ARG:HA	1.81	0.42
1:A:454:LYS:HZ1	1:A:552:VAL:HB	1.84	0.41
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.92	0.41
2:B:394:GLN:OE1	2:B:418:ASN:ND2	2.51	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.56	0.41
2:B:354:TYR:OH	2:B:378:GLU:OE2	2.35	0.41
2:B:362:THR:OG1	2:B:362:THR:O	2.38	0.40
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.96	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:LEU:HB3	1:A:214:LEU:HB2	2.03	0.40
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.22	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	552/557 (99%)	529 (96%)	19 (3%)	4 (1%)	30	34
2	B	408/428 (95%)	388 (95%)	18 (4%)	2 (0%)	38	45
All	All	960/985 (98%)	917 (96%)	37 (4%)	6 (1%)	33	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	PRO
1	A	545	ASN
1	A	285	GLY
2	B	272	PRO
1	A	286	THR
2	B	86	ASP

### 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	494/495 (100%)	472 (96%)	22 (4%)	38	50
2	B	374/390 (96%)	360 (96%)	14 (4%)	45	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	868/885 (98%)	832 (96%)	36 (4%)	41 55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	22	LYS
1	A	67	ASP
1	A	73	LYS
1	A	101	LYS
1	A	105	SER
1	A	161	GLN
1	A	162	SER
1	A	184	MET
1	A	195	ILE
1	A	211	ARG
1	A	221	HIS
1	A	222	GLN
1	A	286	THR
1	A	290	THR
1	A	300	GLU
1	A	324	ASP
1	A	349	LEU
1	A	399	GLU
1	A	503	LEU
1	A	514	GLU
1	A	546	GLU
2	B	8	VAL
2	B	66	LYS
2	B	87	PHE
2	B	90	VAL
2	B	165	THR
2	B	210	LEU
2	B	214	LEU
2	B	227	PHE
2	B	228	LEU
2	B	238	LYS
2	B	356	ARG
2	B	362	THR
2	B	417	VAL
2	B	425	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	G73	A	601	-	34,34,34	1.47	3 (8%)	45,47,47	5.11	6 (13%)

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	G73	A	601	-	-	0/14/14/14	0/2/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	G73	C12-N13	5.33	1.44	1.36
3	A	601	G73	C10-N09	4.16	1.44	1.36
3	A	601	G73	C27-N31	3.21	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	G73	N31-C27-N26	32.65	134.24	128.18
3	A	601	G73	C28-C27-N26	-4.82	118.95	125.94
3	A	601	G73	C12-N26-C27	4.61	120.94	115.15
3	A	601	G73	N26-C12-N11	-3.76	120.38	126.19
3	A	601	G73	C12-N11-C10	2.58	122.33	116.97
3	A	601	G73	C30-N31-C27	2.48	108.73	103.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	554/557 (99%)	0.45	49 (8%) 10 16	25, 46, 86, 129	0
2	B	412/428 (96%)	0.83	60 (14%) 3 5	26, 47, 95, 125	0
All	All	966/985 (98%)	0.61	109 (11%) 6 9	25, 47, 92, 129	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	11.8
1	A	67	ASP	9.2
2	B	88	TRP	8.7
2	B	357	MET	8.3
2	B	214	LEU	8.0
2	B	229	TRP	7.9
2	B	227	PHE	7.7
1	A	219	LYS	7.5
1	A	552	VAL	7.1
1	A	551	LEU	6.9
1	A	220	LYS	6.8
2	B	92	LEU	6.8
1	A	286	THR	6.7
2	B	93	GLY	6.4
2	B	240	THR	6.2
1	A	221	HIS	6.0
1	A	24	TRP	6.0
2	B	91	GLN	5.8
2	B	168	LEU	5.7
1	A	218	ASP	5.5
2	B	231	GLY	5.2
1	A	287	LYS	5.1
2	B	212	TRP	4.9
1	A	290	THR	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	87	PHE	4.6
2	B	89	GLU	4.6
2	B	173	LYS	4.5
2	B	209	LEU	4.5
2	B	170	PRO	4.3
1	A	358	ARG	4.3
1	A	285	GLY	4.2
2	B	210	LEU	4.2
1	A	69	THR	4.1
2	B	230	MET	4.0
2	B	95	PRO	4.0
1	A	288	ALA	3.9
1	A	292	VAL	3.8
2	B	171	PHE	3.8
1	A	293	ILE	3.8
1	A	284	ARG	3.6
1	A	548	VAL	3.5
2	B	86	ASP	3.5
2	B	206	ARG	3.5
2	B	94	ILE	3.4
2	B	228	LEU	3.4
2	B	15	GLY	3.4
2	B	196	GLY	3.3
1	A	289	LEU	3.3
1	A	66	LYS	3.3
2	B	356	ARG	3.3
2	B	204	GLU	3.2
1	A	295	LEU	3.2
2	B	11	LYS	3.1
2	B	358	ARG	3.1
1	A	70	LYS	3.1
2	B	69	THR	3.1
2	B	207	GLN	3.1
2	B	241	VAL	3.0
1	A	63	ILE	3.0
2	B	202	ILE	3.0
1	A	68	SER	3.0
2	B	14	PRO	3.0
1	A	72	ARG	3.0
2	B	277	ARG	3.0
1	A	282	LEU	3.0
2	B	166	LYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	238	LYS	2.9
1	A	252	TRP	2.8
2	B	205	LEU	2.8
1	A	217	PRO	2.7
1	A	544	GLY	2.7
2	B	66	LYS	2.7
1	A	91	GLN	2.7
1	A	257	ILE	2.7
2	B	85	GLN	2.7
1	A	6	GLU	2.6
2	B	167	ILE	2.6
2	B	180	ILE	2.6
2	B	12	LEU	2.6
2	B	284	ARG	2.6
1	A	65	LYS	2.5
2	B	239	TRP	2.4
1	A	64	LYS	2.4
2	B	9	PRO	2.4
2	B	211	ARG	2.4
2	B	193	LEU	2.4
2	B	361	HIS	2.4
1	A	547	GLN	2.4
2	B	197	GLN	2.4
2	B	232	TYR	2.3
1	A	216	THR	2.3
2	B	6	GLU	2.3
1	A	260	LEU	2.3
1	A	114	ALA	2.3
1	A	74	LEU	2.2
1	A	550	LYS	2.2
1	A	14	PRO	2.1
1	A	71	TRP	2.1
2	B	5	ILE	2.1
2	B	425	LEU	2.1
1	A	255	ASN	2.1
1	A	199	ARG	2.1
1	A	224	GLU	2.1
1	A	298	GLU	2.1
1	A	279	LEU	2.1
2	B	315	HIS	2.0
1	A	225	PRO	2.0
2	B	172	LYS	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	242	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	G73	A	601	31/31	0.15	-0.01	31,38,49,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.