



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:56 AM GMT

PDB ID : 3LP1
Title : HIV-1 reverse transcriptase with inhibitor
Authors : Yan, Y.; Munshi, S.K.; Prasad, G.S.; Su, H.P.
Deposited on : 2010-02-04
Resolution : 2.23 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

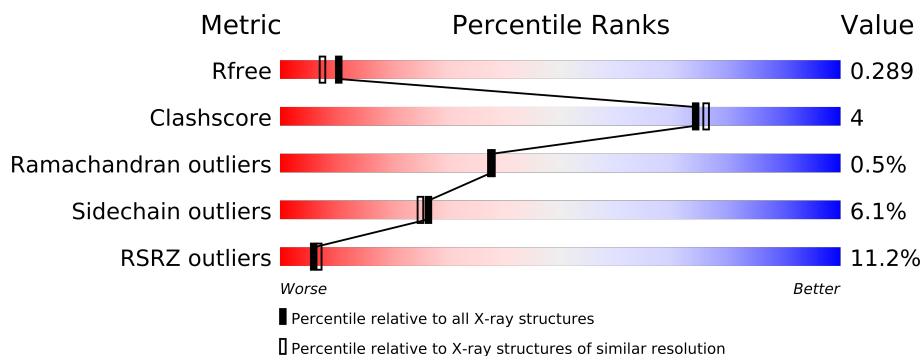
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.23 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	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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 ≥ 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	563	
2	B	443	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8029 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 Reverse transcriptase/ribonucleaseH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4503	2911	751	833	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P04585
A	-1	ASN	-	EXPRESSION TAG	UNP P04585
A	0	SER	-	EXPRESSION TAG	UNP P04585

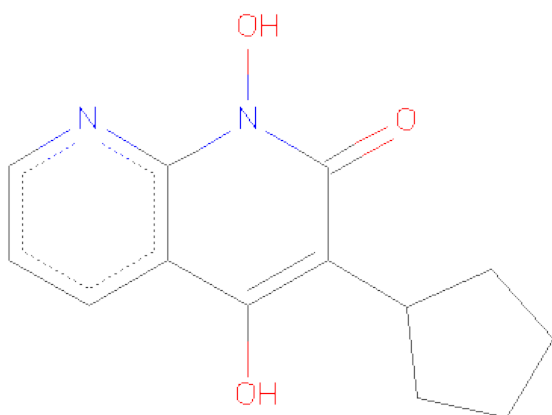
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3311	2155	548	602	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P04585
B	-1	ASN	-	EXPRESSION TAG	UNP P04585
B	0	SER	-	EXPRESSION TAG	UNP P04585

- Molecule 3 is 3-CYCLOPENTYL-1,4-DIHYDROXY-1,8-NAPHTHYRIDIN-2(1H)-ONE (three-letter code: LP8) (formula: C₁₃H₁₄N₂O₃).

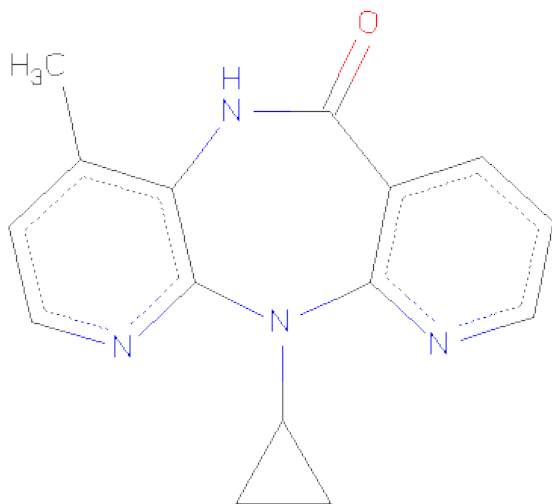


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	13	2	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C₁₅H₁₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total	O	0	0
			108	108		
6	B	67	Total	O	0	0
			67	67		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.78Å 155.26Å 155.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.23 43.06 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.23) 96.2 (43.06-2.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.292 0.266 , 0.289	Depositor DCC
R_{free} test set	3410 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 67665 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: LP8, MN, NVP

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	0.33	0/4619	0.50	0/6279
2	B	0.33	0/3404	0.49	0/4627
All	All	0.33	0/8023	0.50	0/10906

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	4503	0	4540	38	0
2	B	3311	0	3326	28	0
3	A	18	0	12	0	0
4	A	2	0	0	0	0
5	A	20	0	14	1	0
6	A	108	0	0	2	0
6	B	67	0	0	0	0
All	All	8029	0	7892	64	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 4.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.28	0.80
2:B:396:GLU:O	2:B:400:THR:HG22	1.84	0.78
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.32	0.75
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.78	0.65
1:A:91:GLN:HG3	1:A:93:GLY:O	1.97	0.65
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.78	0.64
2:B:373:GLN:O	2:B:377:THR:HG23	1.98	0.64
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.16	0.62
1:A:369:THR:CG2	1:A:398:TRP:HZ3	2.12	0.62
2:B:214:LEU:HD23	2:B:214:LEU:H	1.67	0.60
1:A:199:ARG:HA	1:A:202:ILE:HD12	1.84	0.58
1:A:373:GLN:HG3	6:A:562:HOH:O	2.04	0.57
2:B:388:LYS:HE2	2:B:415:GLU:HG3	1.86	0.57
1:A:91:GLN:HG3	1:A:93:GLY:H	1.69	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.40	0.56
1:A:46:LYS:HE3	1:A:116:PHE:HB3	1.87	0.56
1:A:365:VAL:O	1:A:369:THR:HG23	2.06	0.55
1:A:94:ILE:HD13	1:A:230:MET:HG2	1.90	0.54
1:A:369:THR:HG22	1:A:398:TRP:HZ3	1.72	0.54
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.89	0.53
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.43	0.53
1:A:91:GLN:CG	1:A:93:GLY:O	2.57	0.53
1:A:369:THR:HG22	1:A:398:TRP:CZ3	2.44	0.53
1:A:106:VAL:HG12	1:A:236:PRO:HB3	1.91	0.53
2:B:13:LYS:HE3	2:B:85:GLN:HB3	1.91	0.52
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.91	0.52
2:B:373:GLN:HE22	2:B:407:GLN:H	1.58	0.51
1:A:183:TYR:OH	1:A:230:MET:HE1	2.11	0.51
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.76	0.51
2:B:373:GLN:NE2	2:B:407:GLN:H	2.09	0.50
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.92	0.50
1:A:179:VAL:HG23	5:A:701:NVP:HCC1	1.93	0.50
2:B:345:PRO:O	2:B:346:PHE:HB2	2.10	0.49
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.93	0.49
2:B:362:THR:HG23	2:B:366:LYS:HE3	1.95	0.49
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.95	0.49
1:A:303:LEU:O	1:A:307:ARG:HG3	2.14	0.48
1:A:183:TYR:OH	1:A:230:MET:CE	2.62	0.48
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.78	0.47
1:A:91:GLN:HG2	6:A:573:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.49	0.46
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.98	0.46
2:B:13:LYS:O	2:B:16:MET:HG2	2.16	0.45
2:B:250:ASP:O	2:B:251:SER:HB3	2.17	0.45
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.97	0.45
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.99	0.45
1:A:136:ASN:HB3	1:A:137:ASN:H	1.63	0.45
2:B:58:THR:HG23	2:B:76:ASP:O	2.17	0.44
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.54	0.43
1:A:108:VAL:HG22	1:A:188:TYR:CE2	2.54	0.43
1:A:402:TRP:C	1:A:402:TRP:CD1	2.92	0.42
1:A:452:LEU:HD23	1:A:470:THR:HA	2.01	0.42
1:A:230:MET:HA	1:A:230:MET:HE2	2.01	0.42
1:A:547:GLN:HA	1:A:550:LYS:HE2	2.00	0.42
2:B:157:PRO:HG3	2:B:184:MET:HA	2.01	0.42
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.01	0.41
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.86	0.41
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.18	0.41
2:B:365:VAL:O	2:B:369:THR:HG23	2.21	0.41
1:A:485:ALA:O	1:A:489:SER:HB3	2.21	0.41
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.07	0.41
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.91	0.41
1:A:411:ILE:HG22	1:A:412:PRO:O	2.20	0.41
2:B:246:LEU:HA	2:B:247:PRO:HD3	1.92	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	550/563 (98%)	532 (97%)	14 (2%)	4 (1%)	30	28
2	B	392/443 (88%)	377 (96%)	14 (4%)	1 (0%)	50	54
All	All	942/1006 (94%)	909 (96%)	28 (3%)	5 (0%)	38	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	543	GLY
2	B	296	THR
1	A	345	PRO
1	A	287	LYS

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	492/503 (98%)	460 (94%)	32 (6%)	24	22
2	B	364/403 (90%)	344 (94%)	20 (6%)	30	30
All	All	856/906 (94%)	804 (94%)	52 (6%)	26	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	26	LEU
1	A	118	VAL
1	A	139	THR
1	A	161	GLN
1	A	173	LYS
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	220	LYS
1	A	228	LEU
1	A	248	GLU
1	A	260	LEU
1	A	276	VAL
1	A	279	LEU
1	A	284	ARG

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Mol	Chain	Res	Type
1	A	287	LYS
1	A	297	GLU
1	A	303	LEU
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	448	ARG
1	A	479	LEU
1	A	496	VAL
1	A	503	LEU
1	A	523	GLU
1	A	547	GLN
1	A	548	VAL
2	B	6	GLU
2	B	11	LYS
2	B	12	LEU
2	B	26	LEU
2	B	72	ARG
2	B	80	LEU
2	B	91	GLN
2	B	111	VAL
2	B	116	PHE
2	B	120	LEU
2	B	205	LEU
2	B	209	LEU
2	B	212	TRP
2	B	214	LEU
2	B	297	GLU
2	B	347	LYS
2	B	349	LEU
2	B	362	THR
2	B	400	THR
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	103	ASN
1	A	147	ASN
1	A	198	HIS
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	330	GLN
1	A	407	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
2	B	147	ASN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	367	GLN
2	B	373	GLN

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 ⓘ

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
3	LP8	A	601	4	20,20,20	1.52	2 (10%)	25,29,29	1.77	4 (16%)
5	NVP	A	701	-	18,23,23	1.29	2 (11%)	19,34,34	1.87	6 (31%)

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	LP8	A	601	4	-	0/4/11/11	0/1/3/3
5	NVP	A	701	-	-	0/0/6/6	0/0/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	LP8	O3-C	4.69	1.33	1.24
3	A	601	LP8	C4-N	-3.26	1.35	1.38
5	A	701	NVP	CB-CA	2.51	1.53	1.48
5	A	701	NVP	CC-CA	2.47	1.53	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	LP8	C5-C4-N	-5.53	116.62	122.28
3	A	601	LP8	N9-C4-N	4.26	119.97	116.02
5	A	701	NVP	C5-C6-C7	4.21	119.55	116.82
5	A	701	NVP	C6-C7-C2	-3.36	118.09	122.58
5	A	701	NVP	C4-C5-C6	-2.91	117.59	120.12
3	A	601	LP8	O10-C1-C2	2.48	124.63	120.96
5	A	701	NVP	C10-C15-N14	-2.22	120.72	123.55
5	A	701	NVP	CC-CA-N1	-2.12	116.15	118.41
3	A	601	LP8	C15-C11-C12	2.06	106.36	102.30
5	A	701	NVP	C13-N14-C15	2.03	119.48	116.70

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/563 (98%)	0.68	44 (7%) 13 14	27, 44, 56, 62	0
2	B	400/443 (90%)	0.89	63 (15%) 3 2	29, 40, 80, 83	0
All	All	954/1006 (94%)	0.76	107 (11%) 6 7	27, 43, 71, 83	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	LEU	10.2
2	B	90	VAL	8.8
2	B	299	ALA	7.5
2	B	361	HIS	6.1
2	B	298	GLU	6.0
2	B	362	THR	5.7
2	B	309	ILE	5.4
1	A	52	PRO	4.7
1	A	286	THR	4.7
2	B	251	SER	4.6
1	A	69	THR	4.5
2	B	302	GLU	4.3
2	B	6	GLU	4.3
1	A	193	LEU	4.0
2	B	69	THR	4.0
2	B	314	VAL	3.8
2	B	305	GLU	3.8
2	B	92	LEU	3.7
1	A	137	ASN	3.7
2	B	279	LEU	3.7
2	B	311	LYS	3.6
2	B	13	LYS	3.6
2	B	282	LEU	3.5
2	B	297	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	295	LEU	3.5
2	B	310	LEU	3.5
1	A	284	ARG	3.5
2	B	250	ASP	3.5
2	B	252	TRP	3.5
1	A	63	ILE	3.4
2	B	266	TRP	3.4
1	A	24	TRP	3.4
2	B	281	LYS	3.3
2	B	276	VAL	3.3
2	B	246	LEU	3.3
2	B	290	THR	3.3
1	A	118	VAL	3.2
2	B	277	ARG	3.2
1	A	356	ARG	3.2
1	A	70	LYS	3.2
1	A	360	ALA	3.1
2	B	346	PHE	3.1
2	B	257	ILE	3.1
2	B	280	CYS	3.1
2	B	70	LYS	3.1
1	A	51	GLY	3.1
1	A	526	ILE	3.1
2	B	274	ILE	3.0
1	A	426	TRP	3.0
1	A	514	GLU	3.0
2	B	296	THR	3.0
2	B	283	LEU	3.0
1	A	221	HIS	2.9
1	A	195	ILE	2.9
2	B	292	VAL	2.9
1	A	64	LYS	2.9
1	A	220	LYS	2.9
2	B	14	PRO	2.8
1	A	491	LEU	2.8
2	B	278	GLN	2.8
1	A	402	TRP	2.8
1	A	14	PRO	2.7
2	B	249	LYS	2.7
2	B	313	PRO	2.7
1	A	357	MET	2.7
1	A	334	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	304	ALA	2.6
1	A	196	GLY	2.6
2	B	231	GLY	2.6
2	B	308	GLU	2.5
1	A	228	LEU	2.5
2	B	22	LYS	2.5
1	A	225	PRO	2.5
2	B	306	ASN	2.5
1	A	194	GLU	2.4
1	A	359	GLY	2.4
2	B	214	LEU	2.4
2	B	212	TRP	2.3
2	B	288	ALA	2.3
2	B	16	MET	2.3
2	B	293	ILE	2.3
1	A	173	LYS	2.3
1	A	203	GLU	2.3
2	B	9	PRO	2.3
1	A	2	ILE	2.3
1	A	50	ILE	2.3
1	A	199	ARG	2.2
2	B	8	VAL	2.2
2	B	232	TYR	2.2
1	A	71	TRP	2.2
2	B	24	TRP	2.2
1	A	550	LYS	2.2
2	B	272	PRO	2.2
1	A	43	LYS	2.1
2	B	303	LEU	2.1
1	A	523	GLU	2.1
1	A	111	VAL	2.1
1	A	72	ARG	2.1
2	B	247	PRO	2.1
2	B	286	THR	2.1
1	A	219	LYS	2.1
2	B	401	TRP	2.1
2	B	300	GLU	2.0
1	A	105	SER	2.0
2	B	248	GLU	2.0
1	A	202	ILE	2.0
2	B	261	VAL	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MN	A	602	1/1	0.16	0.54	44,44,44,44	0
5	NVP	A	701	20/20	0.15	-0.33	35,35,36,36	0
3	LP8	A	601	18/18	0.12	-0.80	44,44,45,45	0
4	MN	A	603	1/1	0.12	-1.16	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.