



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2014 – 12:58 AM EDT

PDB ID : 4O44
Title : Crystal Structure of HIV-1 Reverse Transcriptase in complex with 4-((4-(methylamino)-6-(3-morpholinopropoxy)-1,3,5-triazin-2-yl)amino)benzonitrile (JLJ529), a non-nucleoside inhibitor
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Deposited on : 2013-12-18
Resolution : 2.89 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>

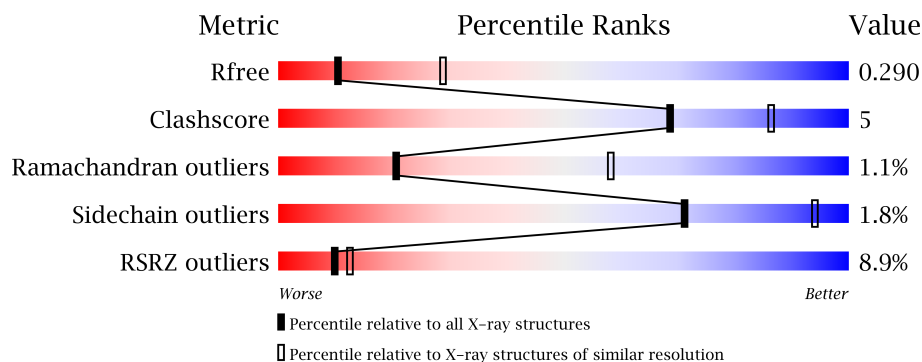
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.89 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	1360 (2.90-2.86)
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (2.90-2.86)
RSRZ outliers	66119	1362 (2.90-2.86)

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	557	
2	B	428	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	2RS	A	601	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8072 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 HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4490	2907	746	830	7			

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

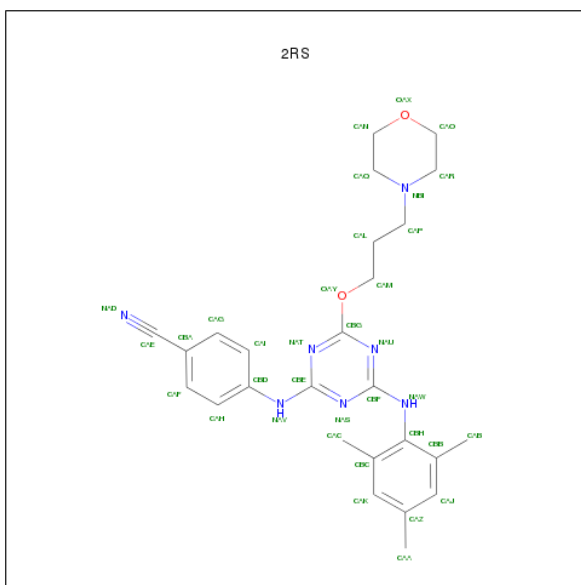
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3529	2300	584	638	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 4-({4-[3-(MORPHOLIN-4-YL)PROPOXY]-6-[(2,4,6-TRIMETHYLPHENYL)AMINO]-1,3,5-TRIAZIN-2-YL}AMINO)BENZONITRILE (three-letter code: 2RS) (formula: C₂₆H₃₁N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	26	7	2		

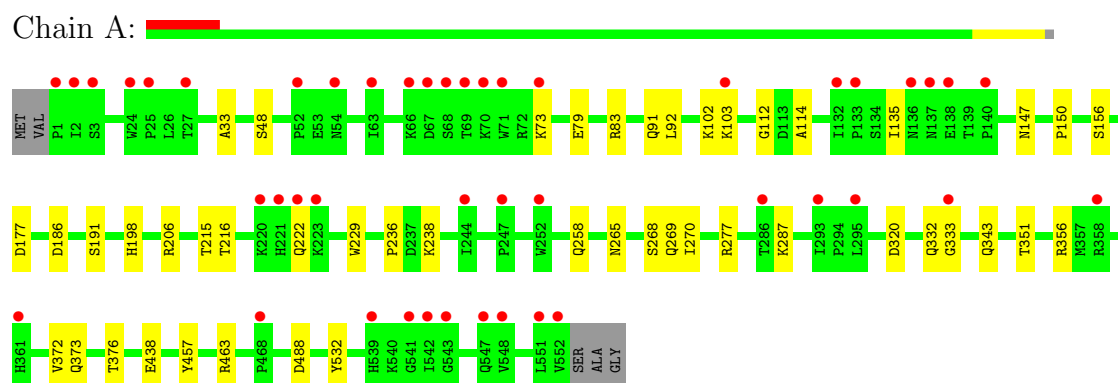
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	8	Total O 8 8	0	0

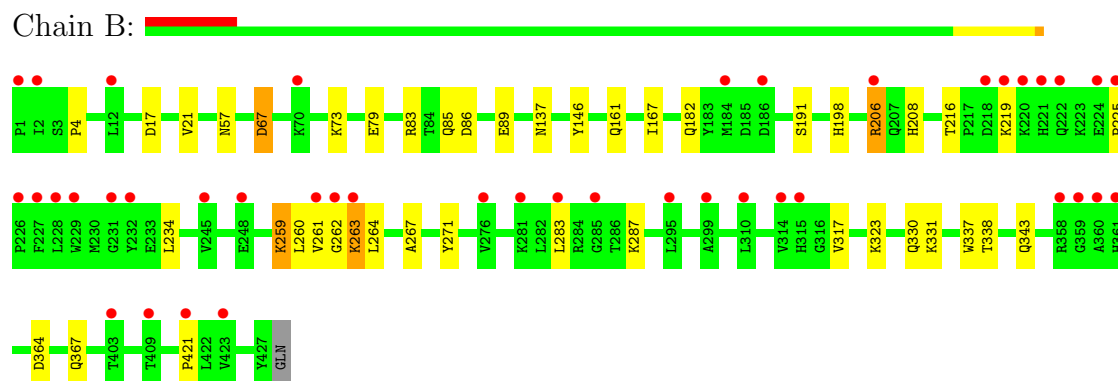
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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 2: HIV-1 reverse transcriptase, p51 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.17Å 69.29Å 104.26Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	36.72 – 2.89 36.72 – 2.89	Depositor EDS
% Data completeness (in resolution range)	90.1 (36.72-2.89) 89.2 (36.72-2.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.233 , 0.290 0.231 , 0.290	Depositor DCC
R_{free} test set	1813 reflections (5.81%)	DCC
Wilson B-factor (Å ²)	86.4	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , -0.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34385 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: 2RS

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	0/4608	0.42	0/6263
2	B	0.26	0/3634	0.45	0/4940
All	All	0.25	0/8242	0.44	0/11203

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	4490	0	0	20	0
2	B	3529	0	5	21	0
3	A	35	0	0	0	0
4	A	10	0	0	1	0
4	B	8	0	0	3	0
All	All	8072	0	5	39	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 (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:191:SER:OG	2:B:198:HIS:ND1	2.26	0.68
1:A:258:GLN:OE1	1:A:287:LYS:NZ	2.28	0.67
2:B:261:VAL:O	2:B:263:LYS:N	2.29	0.65
1:A:206:ARG:NH1	1:A:216:THR:O	2.29	0.64
2:B:263:LYS:O	2:B:267:ALA:N	2.30	0.64
1:A:269:GLN:O	1:A:351:THR:N	2.31	0.63
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.32	0.62
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.32	0.62
1:A:191:SER:OG	1:A:198:HIS:ND1	2.32	0.62
2:B:85:GLN:O	2:B:89:GLU:N	2.35	0.60
2:B:287:LYS:NZ	4:B:508:HOH:O	2.35	0.58
1:A:177:ASP:OD1	1:A:177:ASP:N	2.37	0.57
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.37	0.56
1:A:91:GLN:NE2	2:B:137:ASN:O	2.38	0.56
1:A:238:LYS:NZ	4:A:708:HOH:O	2.37	0.56
1:A:48:SER:OG	1:A:147:ASN:ND2	2.40	0.55
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.41	0.54
1:A:33:ALA:O	1:A:73:LYS:NZ	2.42	0.51
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.43	0.51
2:B:259:LYS:NZ	4:B:505:HOH:O	2.42	0.50
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.30	0.49
1:A:372:VAL:O	1:A:376:THR:OG1	2.32	0.48
2:B:261:VAL:O	2:B:264:LEU:N	2.48	0.46
2:B:21:VAL:O	2:B:57:ASN:ND2	2.49	0.46
1:A:532:TYR:OH	2:B:259:LYS:NZ	2.48	0.46
1:A:265:ASN:O	1:A:268:SER:OG	2.34	0.46
2:B:323:LYS:O	2:B:343:GLN:NE2	2.50	0.45
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.50	0.44
1:A:277:ARG:NH2	1:A:332:GLN:O	2.50	0.44
2:B:17:ASP:N	4:B:506:HOH:O	2.51	0.43
2:B:337:TRP:NE1	2:B:367:GLN:OE1	2.51	0.43
1:A:102:LYS:NZ	1:A:103:LYS:O	2.51	0.43
1:A:102:LYS:NZ	1:A:236:PRO:O	2.52	0.43
2:B:161:GLN:NE2	2:B:182:GLN:OE1	2.52	0.42
2:B:267:ALA:O	2:B:271:TYR:N	2.53	0.42
1:A:320:ASP:O	1:A:343:GLN:NE2	2.53	0.41
2:B:330:GLN:N	2:B:338:THR:O	2.54	0.41
1:A:150:PRO:O	1:A:156:SER:OG	2.39	0.41
2:B:167:ILE:O	2:B:208:HIS:NE2	2.54	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	550/557 (99%)	512 (93%)	33 (6%)	5 (1%)	25	64
2	B	425/428 (99%)	400 (94%)	19 (4%)	6 (1%)	16	50
All	All	975/985 (99%)	912 (94%)	52 (5%)	11 (1%)	21	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	262	GLY
1	A	112	GLY
1	A	114	ALA
1	A	135	ILE
2	B	4	PRO
1	A	229	TRP
2	B	67	ASP
2	B	225	PRO
2	B	263	LYS
2	B	421	PRO
1	A	333	GLY

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	492/495 (99%)	485 (99%)	7 (1%)	78	95
2	B	389/390 (100%)	380 (98%)	9 (2%)	63	91
All	All	881/885 (100%)	865 (98%)	16 (2%)	71	94

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

Mol	Chain	Res	Type
1	A	92	LEU
1	A	186	ASP
1	A	215	THR
1	A	222	GLN
1	A	270	ILE
1	A	356	ARG
1	A	373	GLN
2	B	67	ASP
2	B	86	ASP
2	B	206	ARG
2	B	219	LYS
2	B	234	LEU
2	B	259	LYS
2	B	260	LEU
2	B	283	LEU
2	B	317	VAL

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	2RS	A	601	-	38,38,38	1.56	7 (18%)	51,51,51	2.14	14 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2RS	A	601	-	-	0/17/25/25	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	2RS	OAY-CBG	4.79	1.39	1.34
3	A	601	2RS	CBE-NAV	3.06	1.41	1.36
3	A	601	2RS	CBG-NAT	2.87	1.37	1.33
3	A	601	2RS	CAH-CBD	2.62	1.43	1.39
3	A	601	2RS	CBH-CBB	2.61	1.44	1.40
3	A	601	2RS	CAF-CAH	2.08	1.42	1.38
3	A	601	2RS	CBF-NAW	2.05	1.39	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	2RS	CBG-NAT-CBE	6.02	117.32	112.75
3	A	601	2RS	CBG-NAU-CBF	5.81	117.16	112.75
3	A	601	2RS	CAR-NBI-CAQ	4.56	119.86	108.88
3	A	601	2RS	CBF-NAS-CBE	4.05	119.66	114.05
3	A	601	2RS	NAS-CBE-NAT	-3.48	120.81	126.18
3	A	601	2RS	CAO-CAR-NBI	3.40	114.94	110.08
3	A	601	2RS	NAU-CBG-NAT	-3.40	122.91	127.81
3	A	601	2RS	CAP-NBI-CAQ	3.03	118.86	111.28
3	A	601	2RS	CAN-CAQ-NBI	2.69	113.92	110.08
3	A	601	2RS	NAS-CBF-NAU	-2.62	122.14	126.18
3	A	601	2RS	OAY-CBG-NAT	2.56	124.08	115.88
3	A	601	2RS	CAP-NBI-CAR	2.13	116.61	111.28
3	A	601	2RS	CBD-NAV-CBE	-2.11	123.14	128.97
3	A	601	2RS	CBB-CBH-CBC	-2.05	118.59	121.54

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	552/557 (99%)	0.36	45 (8%) 12 15	25, 57, 147, 218	0
2	B	427/428 (99%)	0.45	42 (9%) 8 10	17, 44, 140, 232	0
All	All	979/985 (99%)	0.40	87 (8%) 10 12	17, 54, 143, 232	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	HIS	15.8
1	A	220	LYS	12.6
2	B	262	GLY	11.1
2	B	222	GLN	10.5
1	A	1	PRO	9.6
2	B	261	VAL	9.5
2	B	360	ALA	9.4
2	B	227	PHE	8.9
1	A	133	PRO	8.6
2	B	1	PRO	7.5
1	A	3	SER	7.0
2	B	226	PRO	6.8
2	B	359	GLY	6.5
1	A	24	TRP	6.4
2	B	218	ASP	6.1
2	B	2	ILE	5.9
2	B	231	GLY	5.7
1	A	52	PRO	5.3
1	A	69	THR	5.3
1	A	552	VAL	5.2
2	B	221	HIS	4.6
1	A	252	TRP	4.6
1	A	541	GLY	4.6
1	A	67	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	358	ARG	4.5
1	A	539	HIS	4.4
1	A	286	THR	4.4
2	B	220	LYS	4.4
1	A	73	LYS	4.3
1	A	222	GLN	4.2
1	A	138	GLU	4.2
2	B	283	LEU	4.2
2	B	225	PRO	4.1
1	A	542	ILE	4.1
1	A	2	ILE	4.0
1	A	548	VAL	3.7
1	A	547	GLN	3.7
2	B	229	TRP	3.7
2	B	219	LYS	3.6
1	A	68	SER	3.4
1	A	25	PRO	3.4
2	B	228	LEU	3.4
1	A	63	ILE	3.4
1	A	361	HIS	3.3
2	B	295	LEU	3.1
1	A	223	LYS	3.1
2	B	314	VAL	3.1
1	A	66	LYS	3.1
2	B	12	LEU	3.0
1	A	140	PRO	2.9
1	A	70	LYS	2.9
1	A	333	GLY	2.9
2	B	315	HIS	2.8
1	A	27	THR	2.8
1	A	244	ILE	2.8
1	A	103	LYS	2.8
2	B	224	GLU	2.8
2	B	245	VAL	2.7
1	A	54	ASN	2.7
2	B	276	VAL	2.7
2	B	409	THR	2.6
2	B	232	TYR	2.6
1	A	247	PRO	2.6
2	B	263	LYS	2.5
2	B	248	GLU	2.4
2	B	403	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	421	PRO	2.4
1	A	136	ASN	2.3
2	B	299	ALA	2.3
2	B	310	LEU	2.3
1	A	71	TRP	2.3
1	A	295	LEU	2.3
1	A	293	ILE	2.3
2	B	281	LYS	2.3
2	B	186	ASP	2.2
1	A	551	LEU	2.2
2	B	361	HIS	2.2
2	B	184	MET	2.2
1	A	137	ASN	2.2
2	B	206	ARG	2.1
1	A	358	ARG	2.1
1	A	132	ILE	2.1
1	A	543	GLY	2.1
2	B	423	VAL	2.1
2	B	285	GLY	2.1
2	B	70	LYS	2.0
1	A	468	PRO	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
3	2RS	A	601	35/35	0.52	3.90	53,63,74,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.