



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:08 AM GMT

PDB ID : 4MFB
Title : Crystal Structure of HIV-1 Reverse Transcriptase in Complex with 8-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)indolizine-2-carbonitrile(JLJ555), a non-nucleoside inhibitor
Authors : Frey, K.M.; Anderson, K.S.
Deposited on : 2013-08-27
Resolution : 2.88 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>

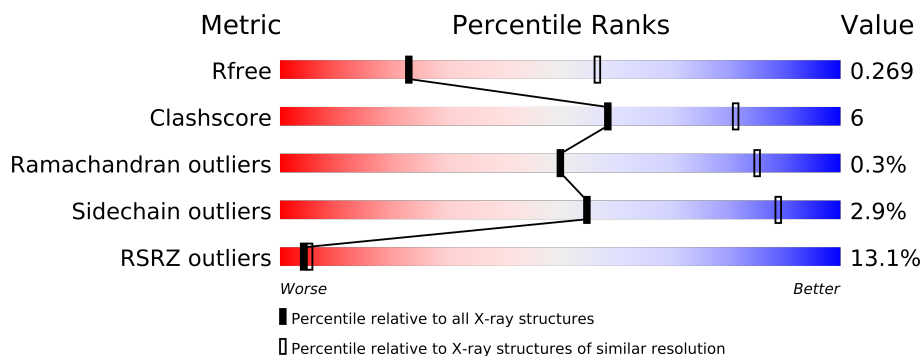
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.88 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	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7877 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	544	Total	C	N	O	S	0	0	0
			4430	2867	737	819	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

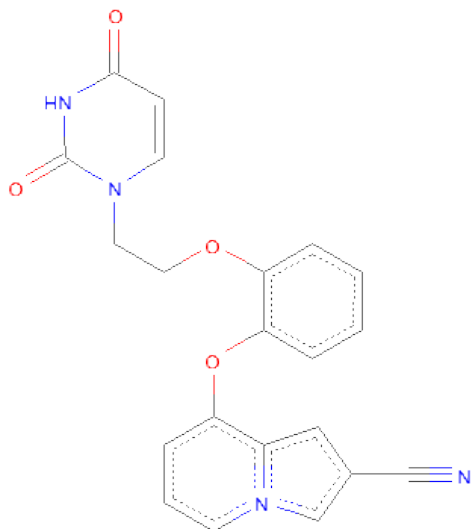
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3401	2211	564	619	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 8-{2-[2-(2,4-DIOXO-3,4-DIHYDROPYRIMIDIN-1(2H)-YL)ETHOXY]PHEN OXY}INDOLIZINE-2-CARBONITRILE (three-letter code: 29T) (formula: C₂₁H₁₆N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	21	4	4		

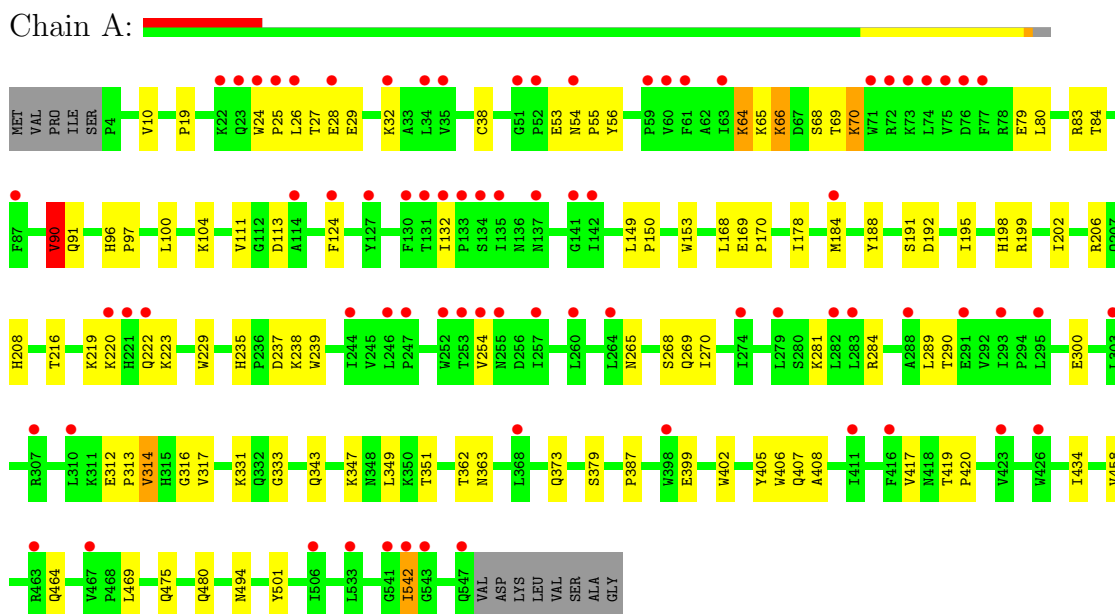
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	10	Total	O	0	0
			10	10		

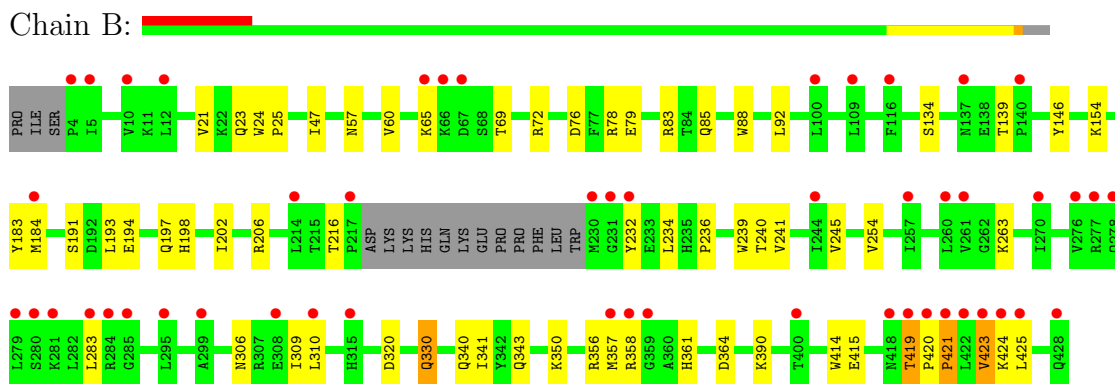
3 Residue-property plots

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 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	223.95Å 69.40Å 104.87Å 90.00° 105.87° 90.00°	Depositor
Resolution (Å)	36.60 – 2.88 49.90 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.60-2.88) 99.1 (49.90-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.269 0.237 , 0.269	Depositor DCC
R_{free} test set	1997 reflections (5.69%)	DCC
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.0	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 35128 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7877	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: 29T

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	0.22	0/4547	0.42	0/6179
2	B	0.22	0/3498	0.44	0/4753
All	All	0.22	0/8045	0.43	0/10932

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	361	HIS	Peptide
2	B	419	THR	Peptide
2	B	421	PRO	Peptide

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	4430	0	4473	60	0
2	B	3401	0	3424	41	0
3	A	29	0	16	6	0
4	A	7	0	0	0	0
4	B	10	0	0	0	0
All	All	7877	0	7913	97	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 6.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:LYS:HG2	1:A:284:ARG:HE	1.57	0.68
2:B:23:GLN:HE22	2:B:60:VAL:H	1.44	0.66
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.77	0.65
2:B:194:GLU:H	2:B:197:GLN:HE21	1.46	0.64
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.80	0.64
2:B:191:SER:OG	2:B:198:HIS:ND1	2.29	0.63
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.62	0.63
1:A:317:VAL:HG11	1:A:347:LYS:HD3	1.80	0.62
1:A:235:HIS:HB2	1:A:238:LYS:HG2	1.82	0.61
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.83	0.61
2:B:65:LYS:HG2	2:B:72:ARG:HB2	1.81	0.61
2:B:320:ASP:O	2:B:343:GLN:NE2	2.25	0.60
1:A:27:THR:OG1	1:A:28:GLU:N	2.35	0.59
1:A:188:TYR:HB3	3:A:601:29T:H6	1.85	0.58
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.36	0.58
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.83	0.58
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.37	0.57
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.37	0.56
1:A:542:ILE:HG22	2:B:283:LEU:HB2	1.88	0.56
2:B:356:ARG:HE	2:B:357:MET:H	1.53	0.54
1:A:281:LYS:HA	1:A:284:ARG:HG3	1.89	0.54
1:A:229:TRP:CG	3:A:601:29T:H2	2.43	0.53
2:B:21:VAL:O	2:B:57:ASN:ND2	2.31	0.53
1:A:195:ILE:O	1:A:199:ARG:HG2	2.08	0.53
1:A:53:GLU:C	1:A:55:PRO:HD3	2.29	0.53
2:B:240:THR:OG1	2:B:241:VAL:N	2.42	0.53
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.91	0.53
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.73	0.52
2:B:193:LEU:HB3	2:B:197:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:245:VAL:O	2:B:263:LYS:NZ	2.41	0.51
1:A:100:LEU:HB3	3:A:601:29T:H11	1.93	0.50
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.93	0.50
1:A:188:TYR:CB	3:A:601:29T:H6	2.41	0.49
1:A:29:GLU:HA	1:A:32:LYS:HD2	1.95	0.49
1:A:191:SER:OG	1:A:198:HIS:ND1	2.33	0.48
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.49	0.48
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.95	0.48
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.48	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.48
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.29	0.48
2:B:194:GLU:HB3	2:B:197:GLN:HG2	1.96	0.47
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.96	0.47
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.49	0.47
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.96	0.47
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.50	0.47
1:A:65:LYS:HG2	1:A:66:LYS:H	1.79	0.47
1:A:254:VAL:HB	1:A:289:LEU:O	2.15	0.47
1:A:90:VAL:HG23	1:A:91:GLN:H	1.80	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.96	0.46
1:A:239:TRP:O	1:A:316:GLY:N	2.44	0.46
1:A:434:ILE:H	1:A:494:ASN:HD21	1.63	0.46
1:A:269:GLN:O	1:A:351:THR:N	2.42	0.46
1:A:417:VAL:HG12	1:A:419:THR:H	1.81	0.45
2:B:341:ILE:HB	2:B:350:LYS:HB3	1.99	0.45
1:A:265:ASN:O	1:A:268:SER:OG	2.26	0.45
2:B:92:LEU:HD12	2:B:92:LEU:HA	1.85	0.45
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.53	0.44
1:A:69:THR:HG23	1:A:70:LYS:HD2	2.00	0.44
1:A:229:TRP:CD2	3:A:601:29T:H2	2.52	0.44
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.53	0.44
2:B:423:VAL:HG23	2:B:424:LYS:H	1.83	0.44
2:B:134:SER:OG	2:B:139:THR:O	2.24	0.43
2:B:234:LEU:HD13	2:B:239:TRP:HH2	1.82	0.43
1:A:202:ILE:O	1:A:206:ARG:HG3	2.19	0.43
1:A:406:TRP:CH2	2:B:420:PRO:HD2	2.54	0.43
2:B:198:HIS:O	2:B:202:ILE:HG12	2.19	0.43
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.54	0.43
1:A:270:ILE:HG13	1:A:314:VAL:HG13	2.00	0.43
1:A:79:GLU:O	1:A:83:ARG:NH1	2.50	0.42
2:B:183:TYR:CD2	2:B:184:MET:HG2	2.53	0.42
1:A:229:TRP:CD1	3:A:601:29T:H2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:330:GLN:OE1	2:B:340:GLN:NE2	2.32	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD2	1.66	0.42
1:A:25:PRO:HA	1:A:26:LEU:HA	1.81	0.42
2:B:306:ASN:O	2:B:310:LEU:HB2	2.20	0.42
2:B:423:VAL:HG23	2:B:424:LYS:N	2.35	0.42
2:B:357:MET:HG3	2:B:358:ARG:O	2.20	0.42
1:A:170:PRO:HG2	1:A:208:HIS:HE1	1.84	0.42
1:A:19:PRO:O	1:A:56:TYR:HB3	2.20	0.42
2:B:154:LYS:HG2	2:B:184:MET:CE	2.50	0.42
1:A:419:THR:HA	1:A:420:PRO:HD3	1.86	0.41
1:A:28:GLU:HB3	1:A:32:LYS:HE3	2.01	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.93	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.93	0.41
1:A:222:GLN:HG3	1:A:223:LYS:HG3	2.01	0.41
1:A:362:THR:OG1	1:A:363:ASN:N	2.54	0.41
2:B:425:LEU:H	2:B:425:LEU:HG	1.63	0.41
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.54	0.41
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.86	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.94	0.40
2:B:356:ARG:HA	2:B:356:ARG:HD2	1.93	0.40
1:A:53:GLU:HG3	1:A:54:ASN:H	1.87	0.40
1:A:64:LYS:HG2	1:A:65:LYS:O	2.21	0.40
2:B:330:GLN:HB3	2:B:330:GLN:HE21	1.76	0.40
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.61	0.40
2:B:24:TRP:HA	2:B:25:PRO:HD3	1.99	0.40
1:A:379:SER:CB	1:A:387:PRO:HD3	2.52	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	542/557 (97%)	522 (96%)	18 (3%)	2 (0%)	43	82
2	B	409/428 (96%)	400 (98%)	8 (2%)	1 (0%)	56	89

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	951/985 (96%)	922 (97%)	26 (3%)	3 (0%)	50 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	423	VAL
1	A	220	LYS
1	A	90	VAL

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	484/495 (98%)	464 (96%)	20 (4%)	41 80
2	B	373/390 (96%)	368 (99%)	5 (1%)	80 96
All	All	857/885 (97%)	832 (97%)	25 (3%)	55 89

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	64	LYS
1	A	66	LYS
1	A	68	SER
1	A	70	LYS
1	A	90	VAL
1	A	111	VAL
1	A	113	ASP
1	A	168	LEU
1	A	169	GLU
1	A	178	ILE
1	A	184	MET
1	A	216	THR
1	A	219	LYS
1	A	237	ASP
1	A	290	THR

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Mol	Chain	Res	Type
1	A	300	GLU
1	A	314	VAL
1	A	373	GLN
1	A	542	ILE
2	B	69	THR
2	B	232	TYR
2	B	330	GLN
2	B	414	TRP
2	B	419	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	208	HIS
1	A	255	ASN
1	A	361	HIS
1	A	474	ASN
2	B	23	GLN
2	B	147	ASN
2	B	197	GLN
2	B	255	ASN

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	29T	A	601	-	32,32,32	1.54	5 (15%)	39,44,44	1.62	7 (17%)

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	29T	A	601	-	-	0/10/12/12	0/2/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	29T	C0P-N0H	6.11	1.43	1.33
3	A	601	29T	C0Y-C0Z	2.68	1.45	1.39
3	A	601	29T	C0O-C0N	2.39	1.46	1.40
3	A	601	29T	C0C-C0V	2.16	1.44	1.41
3	A	601	29T	C0Z-C0C	2.07	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	29T	C0X-N0W-C11	-4.19	124.65	131.04
3	A	601	29T	C0E-N0H-C0K	3.94	124.83	119.69
3	A	601	29T	C0X-N0W-C0V	3.80	126.44	121.51
3	A	601	29T	C0D-C0E-N0H	3.15	115.79	110.97
3	A	601	29T	C10-C14-C16	-2.98	122.71	126.66
3	A	601	29T	C0E-N0H-C0P	-2.27	114.93	117.78
3	A	601	29T	C0C-C0V-N0W	-2.25	115.41	120.68

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	544/557 (97%)	0.78	75 (13%) 4 4	28, 70, 152, 229	0
2	B	413/428 (96%)	0.78	50 (12%) 5 6	24, 59, 155, 291	0
All	All	957/985 (97%)	0.78	125 (13%) 4 5	24, 67, 153, 291	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	12.4
2	B	231	GLY	11.8
2	B	283	LEU	11.2
2	B	66	LYS	11.1
2	B	67	ASP	8.5
1	A	24	TRP	8.3
2	B	279	LEU	8.2
1	A	25	PRO	7.8
1	A	52	PRO	7.0
2	B	232	TYR	6.6
1	A	221	HIS	6.3
1	A	134	SER	6.1
1	A	260	LEU	6.0
1	A	26	LEU	5.9
1	A	283	LEU	5.7
2	B	4	PRO	5.6
1	A	257	ILE	5.2
1	A	130	PHE	5.2
1	A	252	TRP	5.2
1	A	426	TRP	5.0
2	B	425	LEU	4.9
2	B	424	LYS	4.9
1	A	282	LEU	4.9
2	B	359	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	281	LYS	4.8
1	A	142	ILE	4.7
2	B	277	ARG	4.6
1	A	63	ILE	4.6
2	B	230	MET	4.4
1	A	60	VAL	4.4
1	A	23	GLN	4.4
1	A	279	LEU	4.4
1	A	293	ILE	4.3
2	B	299	ALA	4.2
1	A	247	PRO	4.1
1	A	295	LEU	4.1
2	B	428	GLN	4.1
1	A	22	LYS	4.1
1	A	61	PHE	4.1
1	A	542	ILE	4.0
2	B	310	LEU	4.0
2	B	284	ARG	3.9
2	B	285	GLY	3.9
2	B	276	VAL	3.9
2	B	261	VAL	3.8
2	B	422	LEU	3.7
1	A	72	ARG	3.5
1	A	467	VAL	3.5
1	A	254	VAL	3.4
1	A	222	GLN	3.4
1	A	506	ILE	3.4
1	A	34	LEU	3.4
2	B	420	PRO	3.4
1	A	51	GLY	3.4
1	A	59	PRO	3.4
1	A	246	LEU	3.2
1	A	132	ILE	3.2
1	A	54	ASN	3.2
2	B	280	SER	3.2
2	B	295	LEU	3.2
2	B	260	LEU	3.2
2	B	358	ARG	3.2
1	A	291	GLU	3.1
2	B	257	ILE	3.1
2	B	109	LEU	3.1
1	A	423	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	65	LYS	3.0
1	A	71	TRP	3.0
2	B	116	PHE	3.0
1	A	303	LEU	3.0
1	A	244	ILE	3.0
2	B	357	MET	2.9
2	B	217	PRO	2.9
1	A	288	ALA	2.9
1	A	76	ASP	2.9
2	B	100	LEU	2.9
1	A	75	VAL	2.8
2	B	140	PRO	2.8
2	B	278	GLN	2.8
1	A	135	ILE	2.8
1	A	74	LEU	2.8
1	A	124	PHE	2.7
1	A	411	ILE	2.7
1	A	416	PHE	2.7
1	A	127	TYR	2.7
1	A	131	THR	2.6
1	A	533	LEU	2.6
1	A	541	GLY	2.6
1	A	77	PHE	2.6
2	B	5	ILE	2.6
1	A	253	THR	2.5
2	B	184	MET	2.5
2	B	10	VAL	2.5
1	A	264	LEU	2.5
1	A	73	LYS	2.5
1	A	28	GLU	2.4
2	B	214	LEU	2.4
1	A	137	ASN	2.4
1	A	114	ALA	2.3
2	B	423	VAL	2.3
2	B	419	THR	2.3
1	A	310	LEU	2.3
2	B	421	PRO	2.3
2	B	315	HIS	2.3
1	A	184	MET	2.3
1	A	220	LYS	2.2
2	B	308	GLU	2.2
1	A	274	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	244	ILE	2.2
2	B	418	ASN	2.2
1	A	398	TRP	2.2
1	A	307	ARG	2.2
2	B	12	LEU	2.2
2	B	400	THR	2.2
1	A	35	VAL	2.2
1	A	463	ARG	2.1
1	A	547	GLN	2.1
1	A	141	GLY	2.1
1	A	368	LEU	2.1
2	B	270	ILE	2.1
1	A	543	GLY	2.1
1	A	87	PHE	2.0
2	B	137	ASN	2.0
1	A	255	ASN	2.0
1	A	32	LYS	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	29T	A	601	29/29	0.28	1.10	42,52,61,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.