



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:25 pm BST

PDB ID : 4RW8
Title : Crystal Structure of HIV-1 Reverse Transcriptase in complex with (E)-3-(3-chloro-5-(2-(2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy)phenoxy)phenyl)acrylonitrile (JLJ532), a non-nucleoside inhibitor'
Authors : Frey, K.M.; Anderson, K.S.
Deposited on : 2014-12-01
Resolution : 2.88 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

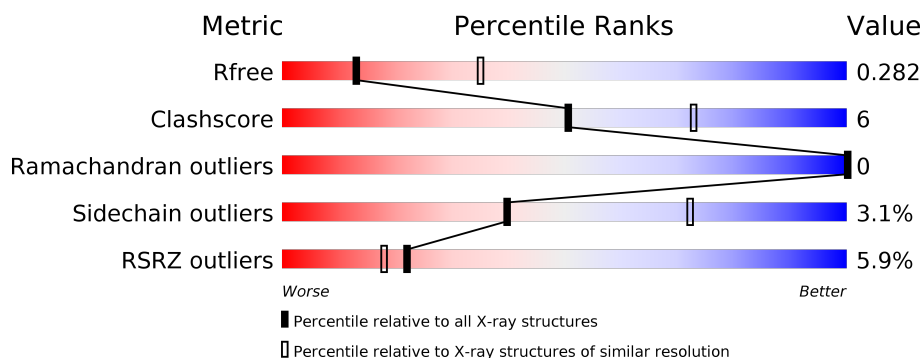
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (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 respectively. 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	557	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>••</div> </div> </div>
2	B	428	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>•</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7930 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 Reverse transcriptase/ribonuclease H, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4458	2886	741	824	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

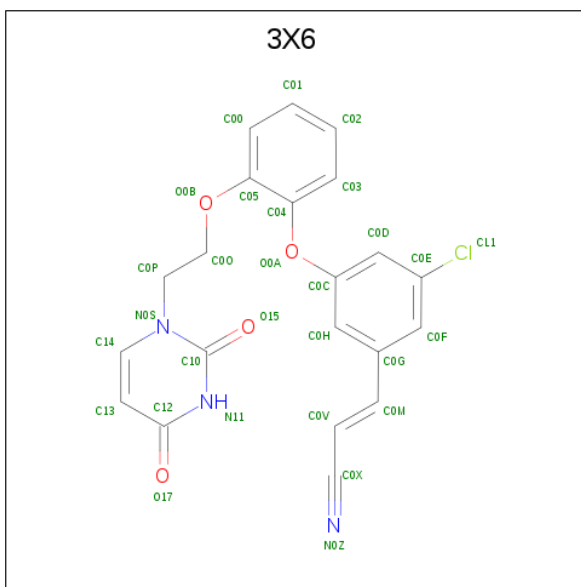
- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	0	0
			3424	2229	566	623	6			

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-(3-chloro-5-{2-[2-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)ethoxy]phenoxy}phenyl)prop-2-enenitrile (three-letter code: 3X6) (formula: C₂₁H₁₆ClN₃O₄).



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

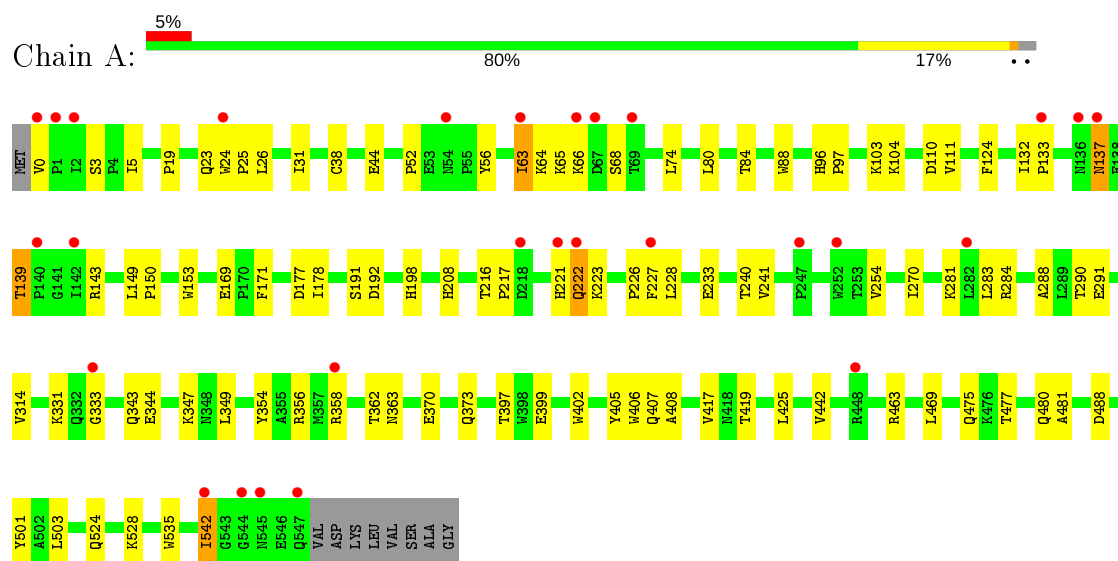
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O		
			8	8	0	0
4	B	11	Total	O		
			11	11	0	0

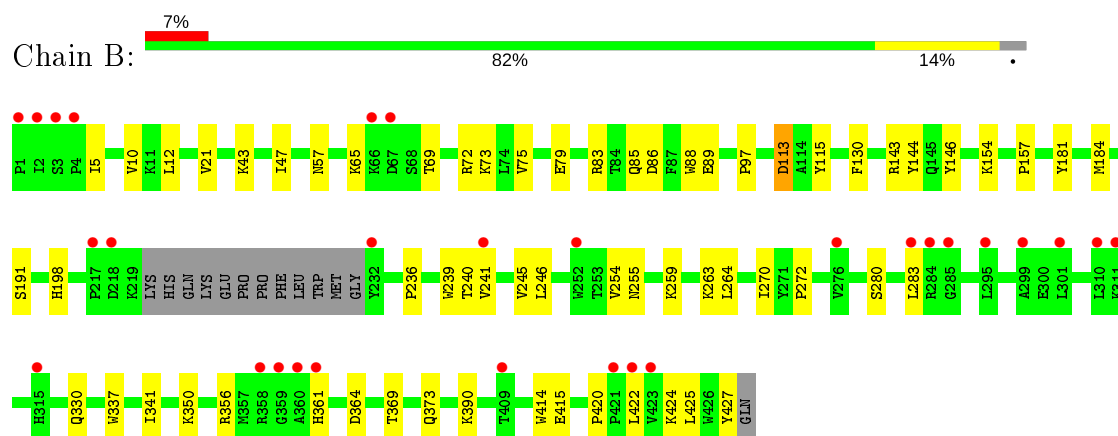
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Reverse transcriptase/ribonuclease H, p66 subunit



- Molecule 2: Reverse transcriptase/ribonuclease H, 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	224.82Å 69.05Å 104.34Å 90.00° 106.29° 90.00°	Depositor
Resolution (Å)	36.60 – 2.88 36.60 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.60-2.88) 99.2 (36.60-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.242 , 0.282 0.242 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3X6

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	0/4576	0.42	0/6221
2	B	0.22	0/3522	0.42	0/4787
All	All	0.22	0/8098	0.42	0/11008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4458	0	4507	63	0
2	B	3424	0	3464	36	0
3	A	29	0	7	0	0
4	A	8	0	0	0	0
4	B	11	0	0	1	0
All	All	7930	0	7978	91	0

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 6.

All (91) 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)
1:A:226:PRO:HA	1:A:227:PHE:HB2	1.52	0.90
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.73	0.70
2:B:85:GLN:O	2:B:89:GLU:N	2.26	0.68
1:A:542:ILE:HG22	2:B:283:LEU:HB2	1.79	0.65
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.80	0.64
2:B:157:PRO:HG3	2:B:184:MET:HA	1.79	0.64
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.80	0.63
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.66	0.61
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.66	0.60
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.85	0.59
1:A:64:LYS:HD2	1:A:68:SER:HA	1.85	0.58
1:A:406:TRP:CG	2:B:420:PRO:HB3	2.39	0.58
1:A:52:PRO:HG3	1:A:143:ARG:HG3	1.86	0.56
1:A:88:TRP:CE2	2:B:143:ARG:HD2	2.40	0.56
1:A:356:ARG:NE	1:A:358:ARG:O	2.40	0.55
1:A:63:ILE:HG22	1:A:64:LYS:H	1.72	0.55
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.71	0.54
1:A:406:TRP:CD2	2:B:420:PRO:HB3	2.43	0.54
2:B:65:LYS:HA	2:B:72:ARG:HD2	1.89	0.54
1:A:191:SER:OG	1:A:198:HIS:ND1	2.32	0.53
2:B:259:LYS:NZ	4:B:509:HOH:O	2.42	0.53
2:B:115:TYR:OH	2:B:184:MET:O	2.25	0.53
2:B:21:VAL:O	2:B:57:ASN:ND2	2.35	0.52
1:A:226:PRO:HB2	1:A:228:LEU:HD12	1.90	0.52
2:B:240:THR:OG1	2:B:241:VAL:N	2.42	0.51
1:A:281:LYS:HG3	1:A:284:ARG:HE	1.75	0.51
1:A:399:GLU:HA	1:A:402:TRP:NE1	2.25	0.51
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.92	0.51
1:A:397:THR:HG23	1:A:425:LEU:HG	1.93	0.51
1:A:417:VAL:HG12	1:A:419:THR:H	1.76	0.50
1:A:64:LYS:NZ	1:A:68:SER:O	2.33	0.50
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.94	0.50
2:B:341:ILE:HB	2:B:350:LYS:HB3	1.94	0.49
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.49
1:A:137:ASN:HB3	1:A:139:THR:HG22	1.95	0.49
1:A:226:PRO:HA	1:A:227:PHE:CB	2.34	0.49
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.47	0.48
2:B:73:LYS:HE2	2:B:75:VAL:HG22	1.96	0.48
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.96	0.47
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.47	0.47
1:A:344:GLU:HB2	1:A:347:LYS:HB2	1.96	0.47
1:A:222:GLN:HB3	1:A:223:LYS:H	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.96	0.47
2:B:97:PRO:HG3	2:B:181:TYR:HB2	1.98	0.46
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.81	0.46
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.97	0.46
1:A:240:THR:OG1	1:A:241:VAL:N	2.49	0.46
1:A:542:ILE:HG23	2:B:280:SER:HA	1.98	0.46
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.46	0.45
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.98	0.45
1:A:217:PRO:HG2	1:A:222:GLN:HG3	1.97	0.45
2:B:245:VAL:O	2:B:263:LYS:NZ	2.36	0.45
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.99	0.45
1:A:25:PRO:HA	1:A:26:LEU:HA	1.74	0.45
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.98	0.45
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.52	0.45
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.22	0.44
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.52	0.44
1:A:463:ARG:NH1	1:A:488:ASP:O	2.51	0.44
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.89	0.43
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.01	0.43
2:B:191:SER:OG	2:B:198:HIS:ND1	2.29	0.43
1:A:0:VAL:HG13	1:A:44:GLU:HA	2.00	0.43
1:A:524:GLN:O	1:A:528:LYS:HG2	2.18	0.43
1:A:233:GLU:HB2	1:A:240:THR:HG23	2.00	0.43
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.59	0.43
1:A:80:LEU:O	1:A:84:THR:HG23	2.19	0.43
1:A:25:PRO:HB2	1:A:26:LEU:HB2	2.00	0.43
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.54	0.43
2:B:113:ASP:N	2:B:113:ASP:OD2	2.41	0.43
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.54	0.43
1:A:406:TRP:CD1	2:B:420:PRO:HB3	2.54	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:177:ASP:OD1	1:A:177:ASP:N	2.49	0.42
1:A:270:ILE:HG13	1:A:314:VAL:HG13	2.00	0.42
1:A:65:LYS:HG2	1:A:66:LYS:H	1.83	0.42
2:B:246:LEU:HD11	2:B:264:LEU:HD21	2.02	0.42
2:B:43:LYS:HB2	2:B:43:LYS:HE3	1.85	0.42
1:A:331:LYS:HG2	1:A:333:GLY:H	1.85	0.41
2:B:255:ASN:O	2:B:259:LYS:HG2	2.20	0.41
2:B:424:LYS:HB3	2:B:425:LEU:H	1.49	0.41
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.55	0.41
1:A:19:PRO:O	1:A:56:TYR:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HB3	1:A:291:GLU:HB2	2.03	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.93	0.41
1:A:3:SER:HB3	1:A:5:ILE:HG13	2.03	0.41
2:B:270:ILE:O	2:B:272:PRO:HD3	2.20	0.41
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.35	0.41
1:A:23:GLN:NE2	1:A:25:PRO:HG2	2.36	0.41
1:A:64:LYS:HD3	1:A:64:LYS:HA	1.95	0.40
1:A:362:THR:OG1	1:A:363:ASN:N	2.55	0.40

There are no symmetry-related clashes.

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	546/557 (98%)	522 (96%)	24 (4%)	0	100	100
2	B	411/428 (96%)	393 (96%)	18 (4%)	0	100	100
All	All	957/985 (97%)	915 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	488/495 (99%)	472 (97%)	16 (3%)	38	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	378/390 (97%)	367 (97%)	11 (3%)	42	74
All	All	866/885 (98%)	839 (97%)	27 (3%)	40	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TRP
1	A	63	ILE
1	A	74	LEU
1	A	103	LYS
1	A	110	ASP
1	A	111	VAL
1	A	137	ASN
1	A	139	THR
1	A	169	GLU
1	A	178	ILE
1	A	216	THR
1	A	221	HIS
1	A	222	GLN
1	A	290	THR
1	A	373	GLN
1	A	542	ILE
2	B	5	ILE
2	B	12	LEU
2	B	69	THR
2	B	86	ASP
2	B	113	ASP
2	B	330	GLN
2	B	356	ARG
2	B	361	HIS
2	B	414	TRP
2	B	422	LEU
2	B	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	GLN
2	B	197	GLN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	548/557 (98%)	0.15	28 (5%)	28 24	36, 74, 123, 159	1 (0%)
2	B	415/428 (96%)	0.24	29 (6%)	16 12	37, 63, 118, 143	1 (0%)
All	All	963/985 (97%)	0.19	57 (5%)	22 18	36, 70, 121, 159	2 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	11.5
2	B	2	ILE	11.3
1	A	1	PRO	7.9
1	A	0	VAL	7.4
1	A	2	ILE	6.8
1	A	24	TRP	5.7
1	A	54	ASN	4.5
1	A	221	HIS	4.3
1	A	133	PRO	4.2
1	A	544	GLY	4.2
1	A	252	TRP	4.1
2	B	284	ARG	4.1
2	B	295	LEU	4.0
1	A	63	ILE	3.8
1	A	137	ASN	3.7
1	A	69	THR	3.7
2	B	358	ARG	3.6
2	B	4	PRO	3.6
1	A	545	ASN	3.4
2	B	315	HIS	3.3
2	B	285	GLY	3.2
2	B	360	ALA	3.2
1	A	222	GLN	3.2
2	B	359	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	3.1
2	B	283	LEU	3.1
1	A	142	ILE	3.0
1	A	448	ARG	3.0
2	B	252	TRP	2.9
1	A	282	LEU	2.9
1	A	66	LYS	2.8
1	A	67	ASP	2.7
2	B	218	ASP	2.6
2	B	232	TYR	2.6
1	A	247	PRO	2.6
1	A	333	GLY	2.5
2	B	276	VAL	2.5
2	B	310	LEU	2.5
2	B	422	LEU	2.4
2	B	3	SER	2.4
2	B	311	LYS	2.4
2	B	299	ALA	2.4
2	B	66	LYS	2.4
2	B	423	VAL	2.3
2	B	409	THR	2.3
1	A	542	ILE	2.3
2	B	421	PRO	2.3
2	B	361	HIS	2.2
1	A	227	PHE	2.2
2	B	301	LEU	2.2
1	A	358	ARG	2.2
2	B	217	PRO	2.2
1	A	140	PRO	2.1
1	A	218	ASP	2.1
2	B	241	VAL	2.0
1	A	136	ASN	2.0
1	A	547	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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3X6	A	601[B]	29/29	0.91	0.26	53,61,74,79	0

6.5 Other polymers

There are no such residues in this entry.