



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2017 – 08:20 PM EDT

PDB ID : 5W86
Title : CRYSTAL STRUCTURE OF JAK3 KINASE DOMAIN WITH A 4,6-DIAMINONICOTINAMIDE INHIBITOR (COMPOUND NUMBER 7)
Authors : Sack, J.S.
Deposited on : unknown
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

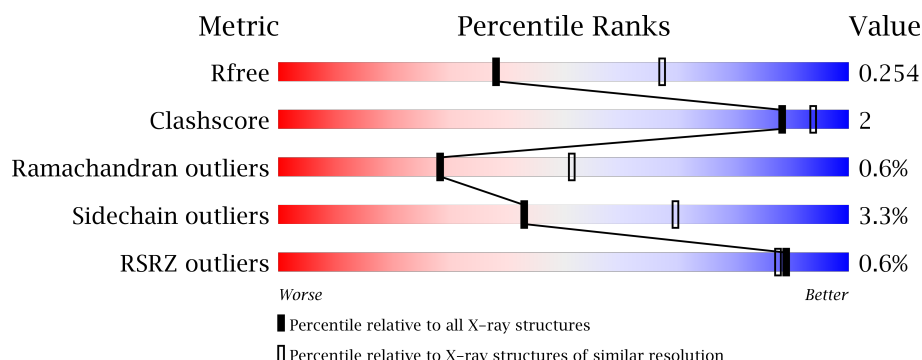
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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. 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	287	<div> <div>90%</div> <div>5% 6%</div> </div>
1	B	287	<div> <div>86%</div> <div>6% • 6%</div> </div>
1	C	287	<div> <div>%</div> <div>87%</div> <div>8% •</div> </div>
1	D	287	<div> <div>%</div> <div>83%</div> <div>12% 5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8915 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.

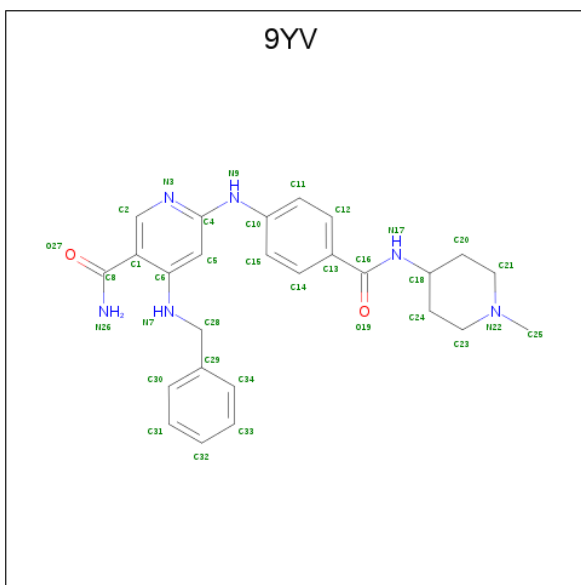
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	P	S	0	1	0
			2126	1358	358	394	2	14			
1	B	269	Total	C	N	O	P	S	0	0	0
			2116	1351	355	394	2	14			
1	C	275	Total	C	N	O	P	S	0	0	0
			2186	1396	374	400	2	14			
1	D	274	Total	C	N	O	P	S	0	0	0
			2196	1401	374	405	2	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1040	SER	CYS	engineered mutation	UNP P52333
A	1048	SER	CYS	engineered mutation	UNP P52333
B	1040	SER	CYS	engineered mutation	UNP P52333
B	1048	SER	CYS	engineered mutation	UNP P52333
C	1040	SER	CYS	engineered mutation	UNP P52333
C	1048	SER	CYS	engineered mutation	UNP P52333
D	1040	SER	CYS	engineered mutation	UNP P52333
D	1048	SER	CYS	engineered mutation	UNP P52333

- Molecule 2 is 4-(benzylamino)-6-({4-[(1-methylpiperidin-4-yl)carbamoyl]phenyl}amino)pyridine-3-carboxamide (three-letter code: 9YV) (formula: C₂₆H₃₀N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	26	6	2		
2	B	1	Total	C	N	O	0	0
			34	26	6	2		
2	C	1	Total	C	N	O	0	0
			34	26	6	2		
2	D	1	Total	C	N	O	0	0
			34	26	6	2		


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	34	Total	O	0	0
			34	34		
3	C	40	Total	O	0	0
			40	40		
3	D	44	Total	O	0	0
			44	44		

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 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.

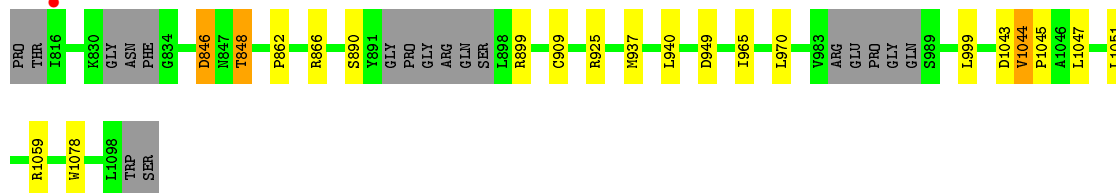
- Molecule 1: Tyrosine-protein kinase JAK3

Chain A: 




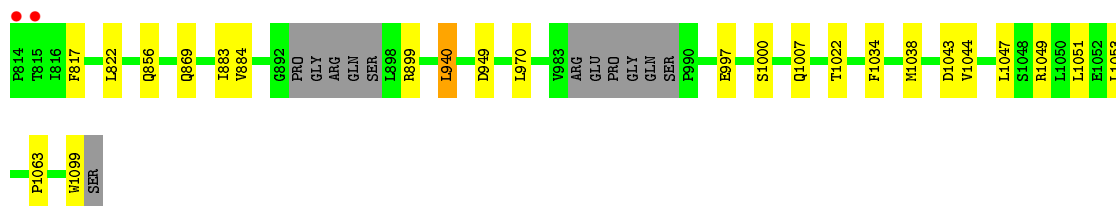
- Molecule 1: Tyrosine-protein kinase JAK3

Chain B: 




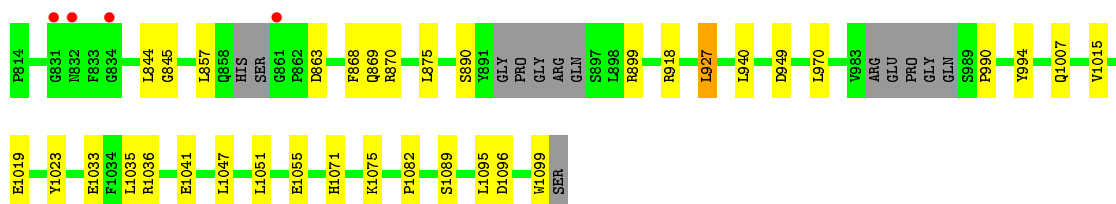
- Molecule 1: Tyrosine-protein kinase JAK3

Chain C: 



- Molecule 1: Tyrosine-protein kinase JAK3

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.98Å 112.30Å 97.12Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	56.98 – 2.61 56.15 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.0 (56.98-2.61) 97.8 (56.15-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.209 , 0.264 0.221 , 0.254	Depositor DCC
R_{free} test set	1824 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.400 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2451e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9YV, PTR

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	0.52	0/2139	0.71	0/2895
1	B	0.53	0/2128	0.70	0/2879
1	C	0.51	0/2203	0.69	0/2978
1	D	0.50	0/2212	0.71	0/2988
All	All	0.52	0/8682	0.70	0/11740

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 [i](#)

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	2126	0	2065	4	0
1	B	2116	0	2056	12	0
1	C	2186	0	2144	10	0
1	D	2196	0	2157	14	0
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	1	0
2	D	34	0	0	0	0
3	A	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	0	0
3	C	40	0	0	0	0
3	D	44	0	0	0	0
All	All	8915	0	8422	40	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 2.

The worst 5 of 40 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:D:1071:HIS:CE1	1:D:1075:LYS:HE2	1.90	1.05
1:C:817:PHE:HB3	1:C:822:LEU:HD11	1.60	0.83
1:B:862:PRO:HB2	1:B:866:ARG:HH21	1.49	0.77
1:D:1033:GLU:OE1	1:D:1036:ARG:NH2	2.23	0.71
1:B:937:MET:CE	1:B:965:ILE:HD13	2.20	0.71

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	261/287 (91%)	249 (95%)	9 (3%)	3 (1%)	17	32
1	B	259/287 (90%)	250 (96%)	8 (3%)	1 (0%)	38	61
1	C	267/287 (93%)	260 (97%)	6 (2%)	1 (0%)	38	61
1	D	264/287 (92%)	253 (96%)	10 (4%)	1 (0%)	38	61
All	All	1051/1148 (92%)	1012 (96%)	33 (3%)	6 (1%)	28	51

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	SER
1	A	1042	ARG
1	B	1043	ASP
1	A	862	PRO
1	C	1043	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	224/249 (90%)	219 (98%)	5 (2%)	57	80
1	B	224/249 (90%)	218 (97%)	6 (3%)	50	76
1	C	232/249 (93%)	224 (97%)	8 (3%)	42	68
1	D	236/249 (95%)	225 (95%)	11 (5%)	30	56
All	All	916/996 (92%)	886 (97%)	30 (3%)	43	69

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	997	GLU
1	C	1047	LEU
1	D	1041	GLU
1	C	1044	VAL
1	C	1053	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1007	GLN
1	D	1071	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are 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
1	PTR	A	980	1	15,16,17	1.02	1 (6%)	19,22,24	0.72	1 (5%)
1	PTR	A	981	1	15,16,17	0.92	1 (6%)	19,22,24	0.75	0
1	PTR	B	980	1	15,16,17	0.75	0	19,22,24	0.47	0
1	PTR	B	981	1	15,16,17	0.79	1 (6%)	19,22,24	0.70	0
1	PTR	C	980	1	15,16,17	0.87	0	19,22,24	0.49	0
1	PTR	C	981	1	15,16,17	0.62	0	19,22,24	0.62	0
1	PTR	D	980	1	15,16,17	0.97	1 (6%)	19,22,24	0.72	0
1	PTR	D	981	1	15,16,17	0.79	1 (6%)	19,22,24	0.85	0

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
1	PTR	A	980	1	-	0/9/11/13	0/1/1/1
1	PTR	A	981	1	-	0/9/11/13	0/1/1/1
1	PTR	B	980	1	-	0/9/11/13	0/1/1/1
1	PTR	B	981	1	-	0/9/11/13	0/1/1/1
1	PTR	C	980	1	-	0/9/11/13	0/1/1/1
1	PTR	C	981	1	-	0/9/11/13	0/1/1/1
1	PTR	D	980	1	-	0/9/11/13	0/1/1/1
1	PTR	D	981	1	-	0/9/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	981	PTR	CA-C	2.09	1.53	1.50
1	B	981	PTR	CA-C	2.17	1.53	1.50
1	A	981	PTR	CA-C	2.52	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	980	PTR	CA-C	2.93	1.54	1.50
1	A	980	PTR	CA-C	3.29	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	PTR	O2P-P-OH	2.09	113.07	105.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	$\# Z > 2$
2	9YV	A	4000	-	37,37,37	0.39	0	47,50,50	0.82	1 (2%)
2	9YV	B	4000	-	37,37,37	0.39	0	47,50,50	0.60	1 (2%)
2	9YV	C	4000	-	37,37,37	0.35	0	47,50,50	0.54	1 (2%)
2	9YV	D	4000	-	37,37,37	0.32	0	47,50,50	0.84	1 (2%)

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
2	9YV	A	4000	-	-	0/21/31/31	0/4/4/4
2	9YV	B	4000	-	-	0/21/31/31	0/4/4/4
2	9YV	C	4000	-	-	0/21/31/31	0/4/4/4
2	9YV	D	4000	-	-	0/21/31/31	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4000	9YV	C6-C1-C8	2.21	123.17	121.75
2	B	4000	9YV	C6-C1-C8	2.51	123.36	121.75
2	A	4000	9YV	C6-C1-C8	4.38	124.56	121.75
2	D	4000	9YV	C6-C1-C8	4.49	124.63	121.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4000	9YV	1	0

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	269/287 (93%)	-0.35	0 100 100	5, 27, 50, 64	13 (4%)
1	B	267/287 (93%)	-0.28	1 (0%) 92 91	11, 30, 49, 67	3 (1%)
1	C	273/287 (95%)	-0.19	2 (0%) 87 85	11, 30, 54, 75	6 (2%)
1	D	272/287 (94%)	-0.15	4 (1%) 74 69	7, 28, 52, 76	6 (2%)
All	All	1081/1148 (94%)	-0.24	7 (0%) 89 87	5, 29, 52, 76	28 (2%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	834	GLY	2.9
1	C	815	THR	2.8
1	D	832	ASN	2.7
1	C	814	PRO	2.6
1	B	816	ILE	2.3

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

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	D	981	16/17	0.91	0.22	-	9,12,25,25	12
1	PTR	A	981	16/17	0.93	0.19	-	12,15,21,23	12
1	PTR	C	981	16/17	0.95	0.16	-	28,30,36,38	12
1	PTR	D	980	16/17	0.88	0.18	-	25,27,31,31	4
1	PTR	C	980	16/17	0.86	0.23	-	36,42,43,44	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PTR	B	980	16/17	0.82	0.20	-	38,42,43,44	4
1	PTR	A	980	16/17	0.89	0.20	-	23,27,29,30	4
1	PTR	B	981	16/17	0.94	0.18	-	26,31,39,41	12

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	9YV	C	4000	34/34	0.95	0.17	1.10	12,19,48,49	0
2	9YV	D	4000	34/34	0.94	0.18	0.95	14,24,61,63	0
2	9YV	A	4000	34/34	0.95	0.15	0.23	7,15,53,54	0
2	9YV	B	4000	34/34	0.94	0.14	-0.39	10,20,40,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.