



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2017 – 04:27 PM EDT

PDB ID : 5UR1
Title : FGFR1 kinase domain complex with SN37333 in reversible binding mode
Authors : Yosaatmadja, Y.; Paik, W.-K.; Smaill, J.B.; Squire, C.J.
Deposited on : 2017-02-09
Resolution : 2.20 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

<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-20029077
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-20029077

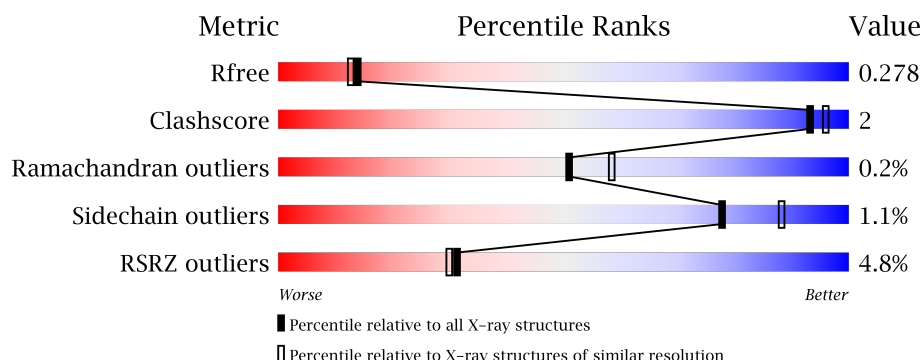
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	311	<div> <div>5%</div> <div>84%</div> <div>6%</div> <div>11%</div> </div>
1	B	311	<div> <div>3%</div> <div>82%</div> <div>•</div> <div>15%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4301 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.

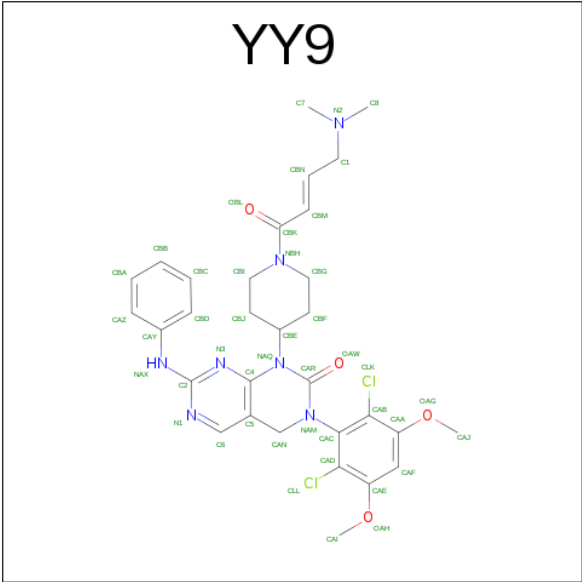
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2140	1359	365	399	17			
1	B	265	Total	C	N	O	S	0	0	0
			2030	1294	345	374	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLY	-	expression tag	UNP P11362
A	456	ALA	-	expression tag	UNP P11362
A	457	MET	-	expression tag	UNP P11362
A	458	SER	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
B	455	GLY	-	expression tag	UNP P11362
B	456	ALA	-	expression tag	UNP P11362
B	457	MET	-	expression tag	UNP P11362
B	458	SER	-	expression tag	UNP P11362
B	488	ALA	CYS	engineered mutation	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362

- Molecule 2 is 3-(2,6-dichloro-3,5-dimethoxyphenyl)-1-{1-[4-(dimethylamino)but-2-enoyl]piperidin-4-yl}-7-(phenylamino)-3,4-dihydropyrimido[4,5-d]pyrimidin-2(1H)-one (three-letter code: YY9) (formula: C₃₁H₃₅Cl₂N₇O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			39	27	2	6	4		
2	B	1	Total	C	Cl	N	O	0	0
			40	28	2	6	4		

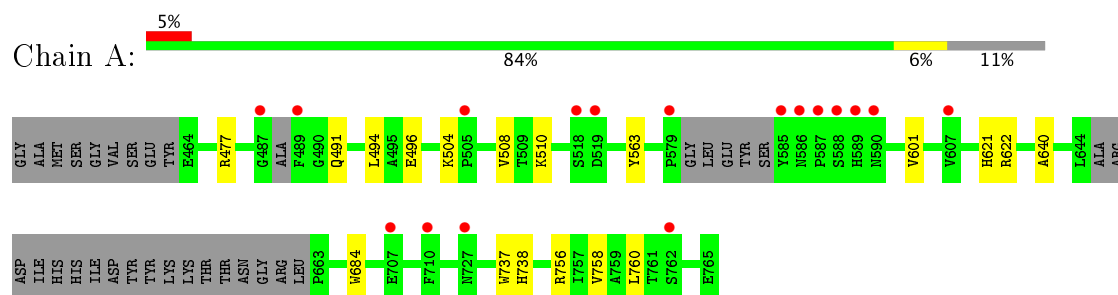
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	24	Total	O	0	0
			24	24		

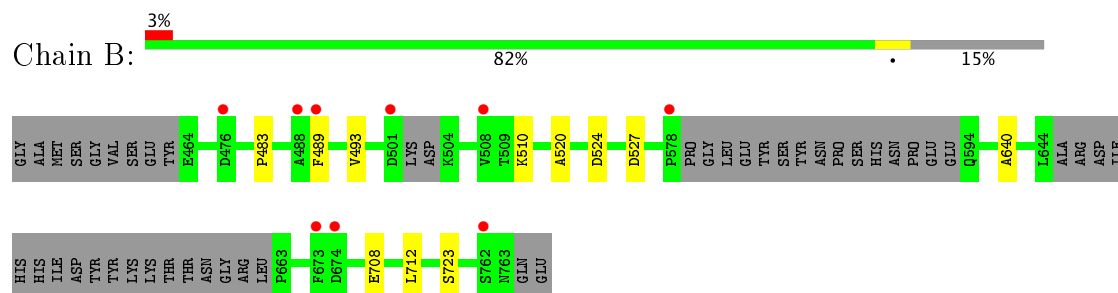
3 Residue-property plots [i](#)

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: Fibroblast growth factor receptor 1



- Molecule 1: Fibroblast growth factor receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.05Å 51.78Å 66.07Å 90.00° 106.87° 90.00°	Depositor
Resolution (Å)	19.54 – 2.20 19.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.54-2.20) 100.0 (19.55-2.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.227 , 0.277 0.232 , 0.278	Depositor DCC
R_{free} test set	1758 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: YY9

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	0.44	0/2183	0.63	0/2961
1	B	0.46	0/2070	0.65	0/2804
All	All	0.45	0/4253	0.64	0/5765

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	2140	0	2077	9	0
1	B	2030	0	1990	5	0
2	A	39	0	0	1	0
2	B	40	0	0	1	0
3	A	28	0	0	0	0
3	B	24	0	0	0	0
All	All	4301	0	4067	14	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.

All (14) 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:B:708:GLU:O	1:B:712:LEU:HD13	2.03	0.58
1:B:640:ALA:HB1	2:B:801:YY9:CLL	2.45	0.52
1:B:483:PRO:HA	1:B:493:VAL:HG12	1.94	0.49
1:A:601:VAL:HG12	1:A:758:VAL:HG23	1.95	0.48
1:B:489:PHE:CD1	1:B:527:ASP:HB3	2.48	0.48
1:A:496:GLU:HB3	1:A:508:VAL:CG1	2.45	0.47
1:A:601:VAL:HG12	1:A:758:VAL:CG2	2.47	0.45
1:A:477:ARG:HA	1:A:477:ARG:NE	2.33	0.44
1:A:684:TRP:CE3	1:A:737:TRP:HA	2.55	0.42
1:A:494:LEU:HD13	1:A:563:TYR:CE1	2.55	0.42
1:A:756:ARG:O	1:A:760:LEU:HD13	2.20	0.42
1:A:640:ALA:HB1	2:A:801:YY9:CLL	2.57	0.41
1:B:520:ALA:HB1	1:B:524:ASP:HB2	2.03	0.41
1:A:621:HIS:O	1:A:622:ARG:HB2	2.21	0.41

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	271/311 (87%)	266 (98%)	4 (2%)	1 (0%)	38	41
1	B	257/311 (83%)	251 (98%)	6 (2%)	0	100	100
All	All	528/622 (85%)	517 (98%)	10 (2%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	LYS

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	224/271 (83%)	221 (99%)	3 (1%)	73	85
1	B	212/271 (78%)	210 (99%)	2 (1%)	82	91
All	All	436/542 (80%)	431 (99%)	5 (1%)	78	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	491	GLN
1	A	510	LYS
1	A	738	HIS
1	B	510	LYS
1	B	723	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	717	HIS

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

2 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	YY9	A	801	-	41,43,48	2.10	8 (19%)	50,62,68	2.36	19 (38%)
2	YY9	B	801	-	42,44,48	2.33	11 (26%)	50,63,68	2.40	20 (40%)

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	YY9	A	801	-	-	0/20/46/52	0/5/5/5
2	YY9	B	801	-	-	0/22/48/52	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	YY9	CAD-CLL	-4.42	1.63	1.72
2	A	801	YY9	CAR-NAM	-2.62	1.34	1.37
2	B	801	YY9	CAR-NAM	-2.19	1.35	1.37
2	B	801	YY9	C6-N1	2.17	1.39	1.34
2	B	801	YY9	CAB-CLK	2.39	1.77	1.72
2	B	801	YY9	CBG-NBH	2.61	1.51	1.47
2	A	801	YY9	CAN-NAM	2.80	1.50	1.46
2	B	801	YY9	CAC-NAM	2.87	1.48	1.44
2	A	801	YY9	CAY-NAX	2.98	1.47	1.40
2	A	801	YY9	CAC-NAM	3.06	1.49	1.44
2	A	801	YY9	CBG-NBH	3.11	1.52	1.47
2	B	801	YY9	CAN-NAM	3.19	1.50	1.46
2	B	801	YY9	CAY-NAX	4.07	1.49	1.40
2	B	801	YY9	CBM-CBK	4.55	1.55	1.48
2	B	801	YY9	CBN-CBM	4.95	1.55	1.30
2	A	801	YY9	C2-NAX	5.16	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	YY9	C2-NAX	5.90	1.47	1.36
2	A	801	YY9	C4-NAQ	8.26	1.49	1.38
2	B	801	YY9	C4-NAQ	8.28	1.49	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	YY9	C4-NAQ-CAR	-7.29	114.70	122.23
2	B	801	YY9	N1-C2-N3	-6.58	120.35	126.68
2	B	801	YY9	C4-NAQ-CAR	-5.93	116.11	122.23
2	A	801	YY9	N1-C2-N3	-5.91	120.99	126.68
2	B	801	YY9	OAW-CAR-NAM	-5.38	114.98	122.02
2	A	801	YY9	CAN-NAM-CAC	-4.77	106.88	116.08
2	B	801	YY9	CAN-NAM-CAC	-3.78	108.78	116.08
2	A	801	YY9	C5-C6-N1	-3.24	118.39	123.87
2	B	801	YY9	CBN-CBM-CBK	-2.92	118.06	121.04
2	A	801	YY9	OAW-CAR-NAM	-2.91	118.22	122.02
2	B	801	YY9	OBL-CBK-CBM	-2.88	116.80	121.20
2	B	801	YY9	CAY-NAX-C2	-2.72	122.08	129.17
2	B	801	YY9	C5-C6-N1	-2.52	119.61	123.87
2	A	801	YY9	CAC-CAD-CLL	-2.25	115.55	119.84
2	A	801	YY9	CBI-NBH-CBK	-2.11	117.28	122.96
2	B	801	YY9	CAA-CAB-CLK	-2.09	115.61	119.42
2	A	801	YY9	CAI-OAH-CAE	-2.06	114.56	117.54
2	A	801	YY9	CBI-CBJ-CBE	-2.01	106.83	110.92
2	A	801	YY9	C2-N3-C4	2.00	121.05	113.95
2	A	801	YY9	NAX-C2-N3	2.06	123.70	116.88
2	B	801	YY9	C6-N1-C2	2.06	119.29	115.88
2	B	801	YY9	NAX-C2-N3	2.11	123.88	116.88
2	B	801	YY9	C2-N3-C4	2.30	122.12	113.95
2	A	801	YY9	N3-C4-NAQ	2.46	120.63	117.49
2	A	801	YY9	C6-N1-C2	2.55	120.10	115.88
2	B	801	YY9	CBF-CBE-NAQ	2.57	120.07	112.31
2	A	801	YY9	CAC-NAM-CAR	2.81	122.25	117.65
2	B	801	YY9	CAC-NAM-CAR	2.88	122.36	117.65
2	A	801	YY9	CAC-CAB-CLK	2.89	125.34	119.84
2	B	801	YY9	C6-C5-C4	3.00	119.57	115.62
2	B	801	YY9	N3-C4-NAQ	3.01	121.33	117.49
2	A	801	YY9	C6-C5-C4	3.22	119.86	115.62
2	B	801	YY9	CBF-CBG-NBH	3.39	115.82	110.82
2	B	801	YY9	CBI-NBH-CBG	3.46	119.14	112.61
2	B	801	YY9	CAC-CAB-CLK	3.70	126.88	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	YY9	CBI-NBH-CBG	4.14	120.44	112.61
2	A	801	YY9	NAQ-CAR-NAM	4.41	122.58	115.65
2	A	801	YY9	CBF-CBG-NBH	4.47	117.40	110.82
2	B	801	YY9	NAQ-CAR-NAM	4.82	123.22	115.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	YY9	1	0
2	B	801	YY9	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	278/311 (89%)	0.15	17 (6%)	22 21	25, 41, 73, 85	0
1	B	265/311 (85%)	0.12	9 (3%)	46 43	25, 40, 64, 81	0
All	All	543/622 (87%)	0.14	26 (4%)	31 30	25, 41, 70, 85	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	762	SER	3.8
1	A	489	PHE	3.7
1	A	589	HIS	3.6
1	A	518	SER	3.4
1	B	489	PHE	3.3
1	A	587	PRO	3.2
1	B	578	PRO	3.2
1	A	590	ASN	3.2
1	A	586	ASN	3.0
1	A	585	TYR	2.8
1	B	488	ALA	2.5
1	A	727	ASN	2.4
1	A	579	PRO	2.4
1	B	501	ASP	2.4
1	A	607	VAL	2.4
1	A	588	SER	2.3
1	A	710	PHE	2.2
1	B	476	ASP	2.1
1	A	505	PRO	2.1
1	A	762	SER	2.1
1	B	674	ASP	2.1
1	A	487	GLY	2.1
1	A	519	ASP	2.1
1	A	707	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	508	VAL	2.0
1	B	673	PHE	2.0

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

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

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(Å ²)	Q<0.9
2	YY9	B	801	40/44	0.91	0.16	0.11	31,36,59,70	0
2	YY9	A	801	39/44	0.93	0.15	-0.04	34,39,60,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.