



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 05:47 AM EST

PDB ID : 5OQ5
Title : Structure of CHK1 8-pt. mutant complex with aminopyrimido-benzodiazepin
one LRRK2 inhibitor
Authors : Dokurno, P.; Williamson, D.S.; Acheson-Dossang, P.; Chen, I.; Murray, J.B.;
Shaw, T.; Surgenor, A.E.
Deposited on : unknown
Resolution : 1.40 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-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

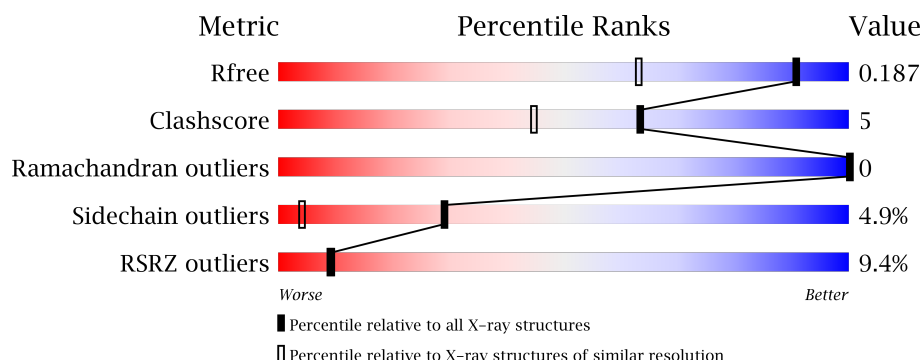
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1307 (1.40-1.40)
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

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	297	<div> <div>8%</div> <div>75%</div> <div>12%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MES	A	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2447 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.

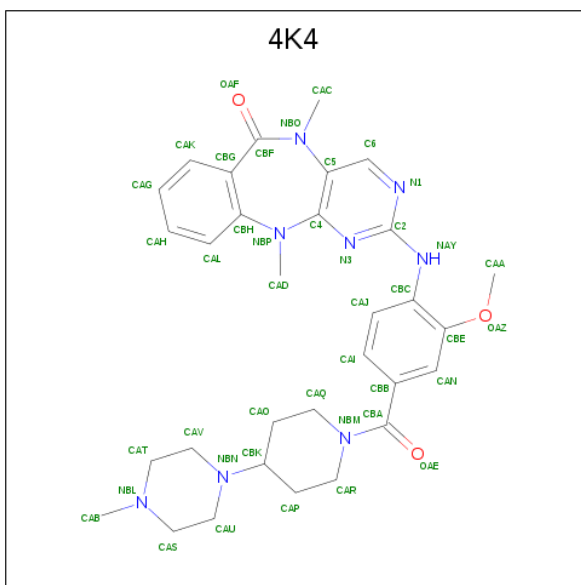
- Molecule 1 is a protein called Serine/threonine-protein kinase Chk1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2106	1350	364	381	11			

There are 16 discrepancies between the modelled and reference sequences:

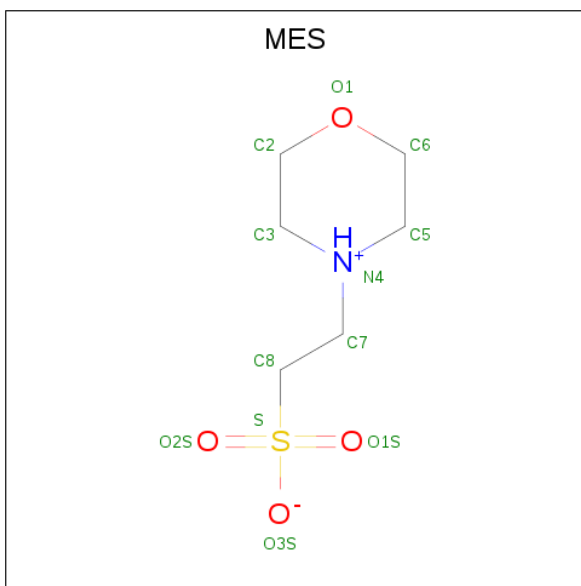
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	LEU	ASN	engineered mutation	UNP O14757
A	68	ILE	VAL	engineered mutation	UNP O14757
A	84	MET	LEU	engineered mutation	UNP O14757
A	86	LEU	TYR	engineered mutation	UNP O14757
A	87	ALA	CYS	engineered mutation	UNP O14757
A	91	SER	GLU	engineered mutation	UNP O14757
A	134	HIS	GLU	engineered mutation	UNP O14757
A	147	ALA	SER	engineered mutation	UNP O14757
A	290	HIS	-	expression tag	UNP O14757
A	291	HIS	-	expression tag	UNP O14757
A	292	HIS	-	expression tag	UNP O14757
A	293	HIS	-	expression tag	UNP O14757
A	294	HIS	-	expression tag	UNP O14757
A	295	HIS	-	expression tag	UNP O14757
A	296	HIS	-	expression tag	UNP O14757
A	297	HIS	-	expression tag	UNP O14757

- Molecule 2 is 2-[(2-methoxy-4-{[4-(4-methylpiperazin-1-yl)piperidin-1-yl]carbonyl}phenyl)amino]-5,11-dimethyl-5,11-dihydro-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one (three-letter code: 4K4) (formula: C₃₁H₃₈N₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	31	8	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total 287	O 287	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.40Å 66.57Å 55.08Å 90.00° 101.58° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 19.86 – 1.40	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-1.40) 96.7 (19.86-1.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.169 , 0.185 0.171 , 0.187	Depositor DCC
R_{free} test set	3013 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2447	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: 4K4, MES

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	1.39	8/2156 (0.4%)	1.35	20/2926 (0.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	TYR	CE1-CZ	7.50	1.48	1.38
1	A	157	TYR	CG-CD2	6.91	1.48	1.39
1	A	104	GLU	CD-OE1	5.59	1.31	1.25
1	A	211	PRO	N-CA	-5.41	1.38	1.47
1	A	219	SER	CA-CB	5.20	1.60	1.52
1	A	236	SER	CB-OG	-5.09	1.35	1.42
1	A	205	GLU	CG-CD	5.06	1.59	1.51
1	A	109	ARG	CZ-NH1	5.03	1.39	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	156	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	157	TYR	CB-CG-CD1	10.08	127.05	121.00
1	A	141	ARG	NE-CZ-NH2	9.42	125.01	120.30
1	A	190	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	263	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	190	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	178	LEU	CB-CG-CD1	6.26	121.64	111.00
1	A	209	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	209	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	181	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	141	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	205	GLU	CG-CD-OE1	-5.67	106.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LEU	CB-CG-CD2	-5.45	101.74	111.00
1	A	139	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	262	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	184	PHE	CB-CG-CD2	5.19	124.43	120.80
1	A	115	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	167	MET	CB-CA-C	-5.06	100.28	110.40
1	A	29	ARG	NE-CZ-NH2	5.05	122.82	120.30

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	2106	0	2079	19	0
2	A	42	0	38	2	0
3	A	12	0	13	0	0
4	A	287	0	0	11	5
All	All	2447	0	2130	21	5

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 5.

All (21) 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:132:LYS:HG3	4:A:402:HOH:O	1.54	1.05
1:A:134:HIS:N	4:A:402:HOH:O	2.01	0.91
1:A:32:GLU:OE1	4:A:403:HOH:O	2.07	0.71
1:A:134:HIS:HB2	4:A:402:HOH:O	1.90	0.71
1:A:213:ASP:HA	4:A:441:HOH:O	1.92	0.68
1:A:10:ASP:OD1	1:A:29:ARG:NH1	2.31	0.63
1:A:180:LYS:HE3	4:A:430:HOH:O	1.99	0.61
1:A:52:ILE:N	1:A:52:ILE:HD12	2.18	0.58
1:A:8:ASP:N	1:A:8:ASP:OD1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASP:OD1	1:A:29:ARG:NE	2.39	0.55
2:A:301:4K4:CAQ	2:A:301:4K4:CAN	2.84	0.55
1:A:162:ARG:NH1	4:A:407:HOH:O	2.38	0.52
1:A:177:GLU:HB2	1:A:181:ARG:HD3	1.95	0.47
2:A:301:4K4:H23	2:A:301:4K4:CAN	2.45	0.45
1:A:260:LYS:HE2	4:A:605:HOH:O	2.15	0.45
1:A:181:ARG:HD2	4:A:626:HOH:O	2.17	0.43
1:A:238:PRO:HD3	1:A:264:TRP:CD1	2.53	0.43
1:A:29:ARG:HG2	4:A:535:HOH:O	2.18	0.42
1:A:140:GLU:OE2	1:A:141:ARG:NH2	2.52	0.42
1:A:141:ARG:HH21	1:A:141:ARG:HG3	1.85	0.42
1:A:68:ILE:HG21	4:A:564:HOH:O	2.20	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:643:HOH:O	4:A:676:HOH:O[2_555]	1.68	0.52
4:A:636:HOH:O	4:A:637:HOH:O[1_554]	1.86	0.34
4:A:581:HOH:O	4:A:597:HOH:O[2_545]	1.94	0.26
4:A:611:HOH:O	4:A:670:HOH:O[2_555]	1.96	0.24
4:A:632:HOH:O	4:A:670:HOH:O[2_555]	2.09	0.11

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	261/297 (88%)	253 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/259 (86%)	213 (95%)	11 (5%)	29 4

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	11	LEU
1	A	13	GLN
1	A	25	LEU
1	A	40	VAL
1	A	78	ASN
1	A	141	ARG
1	A	162	ARG
1	A	174	VAL
1	A	213	ASP
1	A	232	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	78	ASN
1	A	143	ASN
1	A	158	ASN
1	A	165	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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

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	4K4	A	301	-	40,47,47	1.92	11 (27%)	49,68,68	2.00	11 (22%)
3	MES	A	302	-	12,12,12	1.95	4 (33%)	14,16,16	3.23	7 (50%)

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	4K4	A	301	-	-	0/18/38/38	0/5/6/6
3	MES	A	302	-	-	0/6/14/14	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	4K4	CAD-NBP	-4.38	1.43	1.49
2	A	301	4K4	C2-N1	-2.73	1.31	1.34
2	A	301	4K4	C4-N3	-2.17	1.32	1.35
2	A	301	4K4	CAO-CBK	-2.13	1.46	1.52
2	A	301	4K4	CAH-CAL	2.23	1.41	1.36
3	A	302	MES	O1-C2	2.37	1.52	1.42
3	A	302	MES	O3S-S	2.39	1.55	1.47
3	A	302	MES	O2S-S	2.60	1.52	1.45
2	A	301	4K4	CAP-CAR	2.62	1.59	1.52
2	A	301	4K4	C6-N1	2.74	1.39	1.32
2	A	301	4K4	OAZ-CAA	3.32	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	4K4	CAR-NBM	3.68	1.53	1.47
3	A	302	MES	C8-S	4.14	1.83	1.77
2	A	301	4K4	CAQ-NBM	4.14	1.54	1.47
2	A	301	4K4	CBA-NBM	4.20	1.44	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	MES	O3S-S-C8	-8.20	95.97	106.06
2	A	301	4K4	N1-C2-N3	-4.43	122.23	126.65
2	A	301	4K4	CAG-CAK-CBG	-3.56	114.79	120.81
3	A	302	MES	C7-N4-C5	-2.94	103.72	111.26
2	A	301	4K4	CAJ-CBC-CBE	-2.93	115.37	119.05
3	A	302	MES	O1-C2-C3	-2.77	105.63	111.83
2	A	301	4K4	C6-C5-C4	-2.45	115.33	118.76
2	A	301	4K4	CAH-CAL-CBH	-2.43	114.45	119.33
3	A	302	MES	O2S-S-O1S	-2.16	106.37	113.86
3	A	302	MES	O3S-S-O2S	2.05	116.07	111.37
2	A	301	4K4	CBB-CAN-CBE	2.42	122.87	119.63
2	A	301	4K4	CAH-CAG-CAK	2.49	124.00	120.45
3	A	302	MES	O3S-S-O1S	2.80	117.79	111.37
2	A	301	4K4	CAJ-CBC-NAY	3.53	128.83	121.42
2	A	301	4K4	C2-N3-C4	3.67	119.30	115.11
2	A	301	4K4	CAR-NBM-CAQ	3.75	119.70	112.61
3	A	302	MES	O2S-S-C8	5.68	111.67	106.79
2	A	301	4K4	CAK-CBG-CBH	6.97	121.25	118.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	4K4	2	0

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	265/297 (89%)	0.42	25 (9%) 9 9	14, 26, 65, 90	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	VAL	10.1
1	A	48	CYS	9.1
1	A	78	ASN	6.3
1	A	20	TYR	6.2
1	A	18	GLY	6.2
1	A	19	ALA	6.1
1	A	49	PRO	4.7
1	A	44	ARG	4.3
1	A	50	GLU	4.0
1	A	77	GLY	4.0
1	A	42	MET	3.9
1	A	30	VAL	3.9
1	A	213	ASP	3.7
1	A	43	LYS	3.1
1	A	5	PHE	3.1
1	A	6	VAL	3.1
1	A	51	ASN	3.1
1	A	31	THR	3.0
1	A	21	GLY	2.8
1	A	17	GLU	2.6
1	A	27	VAL	2.6
1	A	4	PRO	2.4
1	A	29	ARG	2.3
1	A	68	ILE	2.1
1	A	41	ASP	2.1

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(\AA^2)	Q<0.9
3	MES	A	302	12/12	0.89	0.18	8.45	30,35,48,49	0
2	4K4	A	301	42/42	0.92	0.13	1.91	23,33,69,71	12

6.5 Other polymers [i](#)

There are no such residues in this entry.