



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:11 PM GMT

PDB ID : 4ZY6
Title : Crystal structure of P21-activated kinase 1 in complex with an inhibitor compound 29
Authors : Rouge, L.; Wang, W.
Deposited on : 2015-05-21
Resolution : 2.15 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

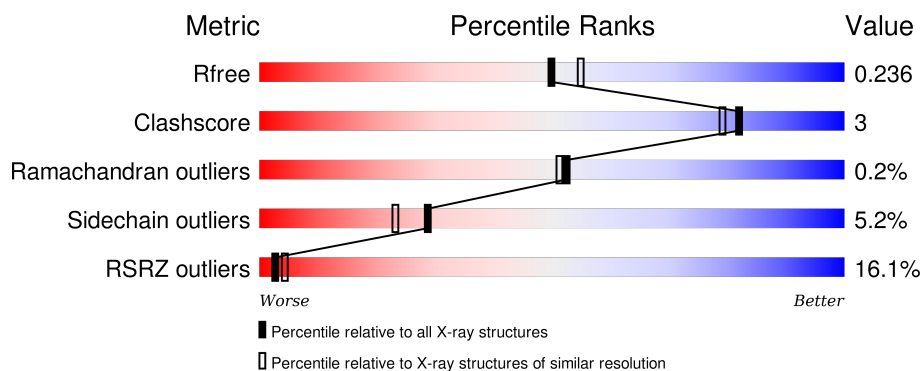
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	301	<div> <div>20%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	B	301	<div> <div>11%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4707 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.

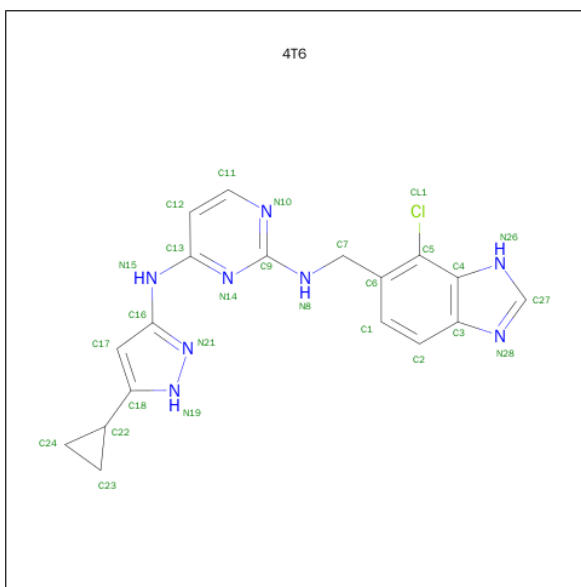
- Molecule 1 is a protein called Serine/threonine-protein kinase PAK 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2229	1419	374	421	15			
1	B	280	Total	C	N	O	S	0	0	0
			2175	1384	364	412	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP Q13153
A	389	ASN	ASP	engineered mutation	UNP Q13153
A	546	GLY	-	expression tag	UNP Q13153
A	547	ASN	-	expression tag	UNP Q13153
A	548	SER	-	expression tag	UNP Q13153
B	248	GLY	-	expression tag	UNP Q13153
B	389	ASN	ASP	engineered mutation	UNP Q13153
B	546	GLY	-	expression tag	UNP Q13153
B	547	ASN	-	expression tag	UNP Q13153
B	548	SER	-	expression tag	UNP Q13153

- Molecule 2 is N 2 -[(7-chloro-1H-benzimidazol-6-yl)methyl]-N 4 -(5-cyclopropyl-1H-pyrazol-3-yl)pyrimidine-2,4-diamine (three-letter code: 4T6) (formula: C₁₈H₁₇ClN₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			27	18	1	8		
2	B	1	Total	C	Cl	N	0	0
			27	18	1	8		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

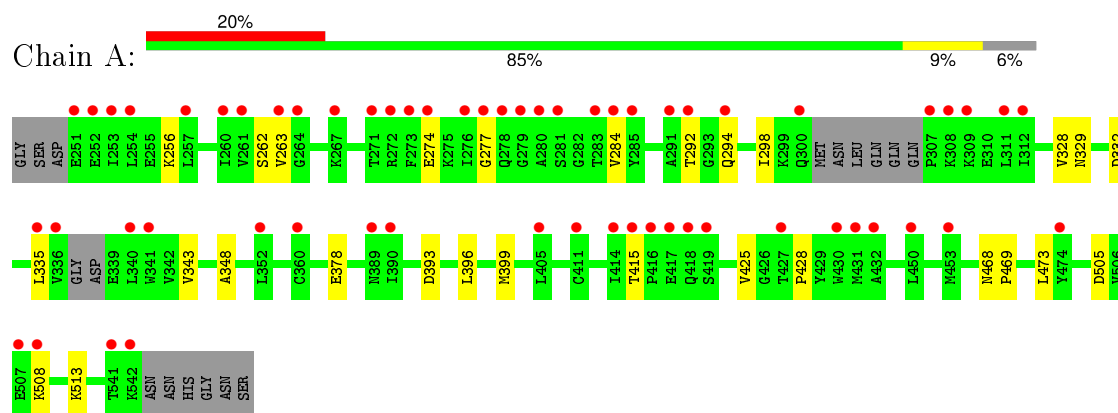
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	139	Total 139	O 139	0	0

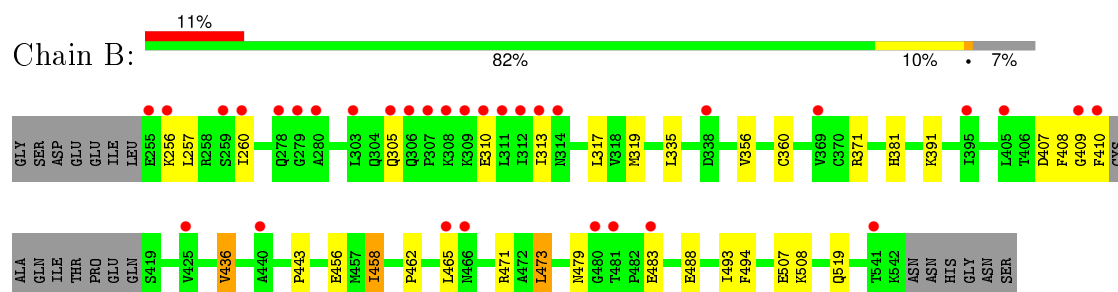
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Serine/threonine-protein kinase PAK 1



- Molecule 1: Serine/threonine-protein kinase PAK 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.63Å 82.24Å 66.14Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	29.36 – 2.15 28.75 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.36-2.15) 99.2 (28.75-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.187 , 0.239 0.183 , 0.236	Depositor DCC
R_{free} test set	1754 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 34882 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4707	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, 4T6

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	0.50	0/2265	0.68	0/3060
1	B	0.53	0/2211	0.66	0/2990
All	All	0.52	0/4476	0.67	0/6050

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	2229	0	2275	12	0
1	B	2175	0	2208	17	0
2	A	27	0	16	1	0
2	B	27	0	16	0	0
3	A	5	0	0	0	0
4	A	105	0	0	1	0
4	B	139	0	0	0	0
All	All	4707	0	4515	29	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 3.

All (29) 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:262:SER:HB3	1:A:263:VAL:HA	1.33	1.04
1:B:409:GLY:HA2	1:B:410:PHE:HB2	1.40	1.04
1:B:408:PHE:N	1:B:409:GLY:HA3	2.06	0.69
1:A:277:GLY:HA3	1:A:284:VAL:H	1.64	0.62
1:B:436:VAL:HG13	1:B:473:LEU:HD13	1.82	0.62
1:A:348:ALA:HB3	1:A:399:MET:HG2	1.84	0.59
1:A:262:SER:HB3	1:A:263:VAL:CA	2.21	0.56
1:B:409:GLY:HA2	1:B:410:PHE:CB	2.24	0.56
1:B:356:VAL:HG11	1:B:456:GLU:HG2	1.87	0.55
1:B:462:PRO:HG2	1:B:465:LEU:HB2	1.89	0.54
1:B:458:ILE:HG12	1:B:494:PHE:CE2	2.43	0.54
1:B:407:ASP:C	1:B:409:GLY:HA3	2.28	0.54
1:B:493:ILE:HD11	1:B:519:GLN:HB2	1.95	0.49
1:A:329:ASN:HA	4:A:744:HOH:O	2.12	0.47
1:B:458:ILE:HG12	1:B:494:PHE:HE2	1.78	0.47
1:A:284:VAL:HG21	2:A:601:4T6:CL1	2.55	0.43
1:B:381:HIS:CG	1:B:443:PRO:HB3	2.53	0.43
1:B:371:ARG:HH11	1:B:371:ARG:HG2	1.83	0.43
1:A:505:ASP:HB3	1:A:508:LYS:HB2	2.01	0.43
1:B:408:PHE:N	1:B:409:GLY:CA	2.80	0.43
1:A:292:THR:OG1	1:A:294:GLN:HG2	2.18	0.43
1:B:409:GLY:CA	1:B:410:PHE:HB2	2.29	0.42
1:B:256:LYS:HE3	1:B:317:LEU:HD11	2.01	0.42
1:A:262:SER:CB	1:A:263:VAL:HA	2.24	0.42
1:A:428:PRO:HG2	1:A:469:PRO:HB3	2.02	0.41
1:B:483:GLU:H	1:B:483:GLU:CD	2.24	0.41
1:A:328:VAL:HG21	1:A:396:LEU:HD12	2.02	0.41
1:A:298:ILE:HG12	1:A:343:VAL:HG22	2.02	0.41
1:B:257:LEU:HD13	1:B:335:LEU:HD11	2.02	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	279/301 (93%)	264 (95%)	14 (5%)	1 (0%)	39	34
1	B	276/301 (92%)	266 (96%)	10 (4%)	0	100	100
All	All	555/602 (92%)	530 (96%)	24 (4%)	1 (0%)	52	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	LEU

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	245/260 (94%)	235 (96%)	10 (4%)	37	35
1	B	238/260 (92%)	223 (94%)	15 (6%)	22	16
All	All	483/520 (93%)	458 (95%)	25 (5%)	29	23

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

Mol	Chain	Res	Type
1	A	256	LYS
1	A	274	GLU
1	A	332	ASP
1	A	378	GLU
1	A	393	ASP
1	A	415	THR
1	A	425	VAL
1	A	468	ASN
1	A	473	LEU
1	A	513	LYS
1	B	260	ILE
1	B	305	GLN

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Mol	Chain	Res	Type
1	B	310	GLU
1	B	313	ILE
1	B	319	MET
1	B	360	CYS
1	B	391	LYS
1	B	436	VAL
1	B	458	ILE
1	B	471	ARG
1	B	473	LEU
1	B	479	ASN
1	B	488	GLU
1	B	507	GLU
1	B	508	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 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	4T6	A	601	-	28,31,31	1.03	1 (3%)	28,44,44	2.29	7 (25%)
3	SO4	A	602	-	4,4,4	0.16	0	6,6,6	0.13	0
2	4T6	B	601	-	28,31,31	1.09	1 (3%)	28,44,44	2.34	8 (28%)

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	4T6	A	601	-	-	0/11/15/15	0/4/5/5
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
2	4T6	B	601	-	-	0/11/15/15	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	4T6	C9-N8	3.01	1.39	1.34
2	A	601	4T6	C9-N8	3.10	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	4T6	N10-C9-N14	-5.17	121.16	126.66
2	A	601	4T6	N10-C9-N14	-4.86	121.49	126.66
2	B	601	4T6	C12-C11-N10	-4.27	118.88	123.88
2	A	601	4T6	C12-C11-N10	-4.19	118.97	123.88
2	B	601	4T6	C12-C13-N14	-2.29	119.08	123.22
2	B	601	4T6	C1-C2-C3	-2.15	118.49	120.86
2	A	601	4T6	C7-C6-C5	-2.11	118.17	121.22
2	B	601	4T6	C7-C6-C5	-2.08	118.22	121.22
2	A	601	4T6	C12-C13-N14	-2.00	119.61	123.22
2	A	601	4T6	C9-N14-C13	2.01	120.14	116.61
2	A	601	4T6	C23-C22-C24	2.12	60.47	58.73
2	B	601	4T6	C9-N14-C13	2.39	120.81	116.61
2	B	601	4T6	C4-C5-CL1	2.51	121.06	117.56
2	A	601	4T6	C11-N10-C9	7.73	121.39	115.42
2	B	601	4T6	C11-N10-C9	7.84	121.48	115.42

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	A	601	4T6	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	284/301 (94%)	1.05	59 (20%) 1 2	30, 58, 117, 164	0
1	B	280/301 (93%)	0.42	32 (11%) 7 11	29, 48, 97, 138	0
All	All	564/602 (93%)	0.74	91 (16%) 3 4	29, 53, 113, 164	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ILE	11.0
1	B	306	GLN	7.4
1	A	254	LEU	7.1
1	A	257	LEU	6.8
1	A	416	PRO	6.2
1	A	417	GLU	5.8
1	A	280	ALA	5.7
1	A	418	GLN	5.7
1	A	390	ILE	5.5
1	A	251	GLU	5.4
1	A	277	GLY	5.4
1	B	410	PHE	5.4
1	A	271	THR	5.3
1	A	276	ILE	5.3
1	B	307	PRO	5.3
1	A	279	GLY	5.3
1	A	415	THR	5.0
1	B	409	GLY	5.0
1	B	465	LEU	4.9
1	A	340	LEU	4.8
1	A	284	VAL	4.7
1	A	273	PHE	4.4
1	A	307	PRO	4.3
1	A	263	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	308	LYS	4.3
1	A	419	SER	4.3
1	A	252	GLU	4.3
1	B	310	GLU	4.1
1	A	414	ILE	4.0
1	B	313	ILE	3.9
1	A	309	LYS	3.8
1	A	274	GLU	3.7
1	A	260	ILE	3.6
1	A	341	TRP	3.6
1	A	474	TYR	3.6
1	B	256	LYS	3.5
1	B	308	LYS	3.4
1	A	411	CYS	3.2
1	B	260	ILE	3.2
1	B	440	ALA	3.1
1	B	311	LEU	3.1
1	A	312	ILE	3.1
1	A	507	GLU	2.9
1	A	283	THR	2.9
1	B	314	ASN	2.8
1	A	336	VAL	2.8
1	A	281	SER	2.8
1	A	431	MET	2.8
1	A	285	TYR	2.8
1	A	278	GLN	2.8
1	A	272	ARG	2.7
1	A	453	MET	2.6
1	B	259	SER	2.6
1	A	311	LEU	2.6
1	B	369	VAL	2.5
1	A	430	TRP	2.5
1	B	483	GLU	2.5
1	B	303	LEU	2.5
1	B	405	LEU	2.4
1	A	264	GLY	2.4
1	B	481	THR	2.4
1	A	294	GLN	2.4
1	A	405	LEU	2.4
1	A	360	CYS	2.3
1	A	450	LEU	2.3
1	A	261	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	280	ALA	2.3
1	B	305	GLN	2.3
1	A	335	LEU	2.3
1	B	466	ASN	2.3
1	A	291	ALA	2.3
1	A	267	LYS	2.3
1	A	432	ALA	2.2
1	B	309	LYS	2.2
1	A	542	LYS	2.2
1	A	352	LEU	2.2
1	B	395	ILE	2.2
1	A	300	GLN	2.2
1	B	255	GLU	2.2
1	A	389	ASN	2.2
1	B	278	GLN	2.1
1	B	312	ILE	2.1
1	B	338	ASP	2.1
1	A	292	THR	2.1
1	B	480	GLY	2.1
1	A	427	THR	2.1
1	A	541	THR	2.1
1	B	279	GLY	2.1
1	B	425	VAL	2.1
1	A	508	LYS	2.0
1	B	541	THR	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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	4T6	B	601	27/27	0.94	0.12	-0.26	36,46,51,54	0
2	4T6	A	601	27/27	0.95	0.10	-0.74	39,48,53,55	0
3	SO4	A	602	5/5	0.92	0.12	-1.12	102,102,103,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.