W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:25 AM GMT

PDB ID	:	3EN6
Title	:	Targeted polypharmacology: crystal structure of the c-Src kinase domain in complex with PP102, a multitargeted kinase inhibitor
Authors	:	Blair, J.A.; Apsel, B.; Knight, Z.A.; Shokat, K.M.
Deposited on	:	2008-09-25
Resolution	:	2.39 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
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)	:	trunk26865
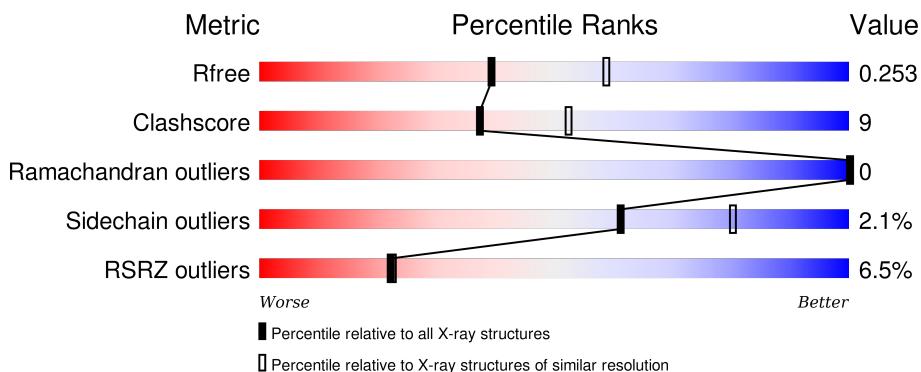
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
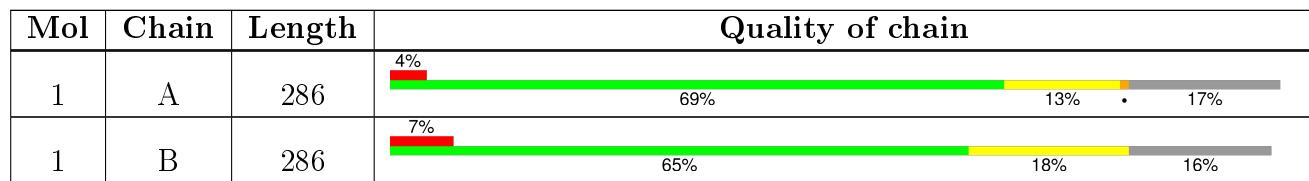
The reported resolution of this entry is 2.39 Å.

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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	286	
1	B	286	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3749 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.
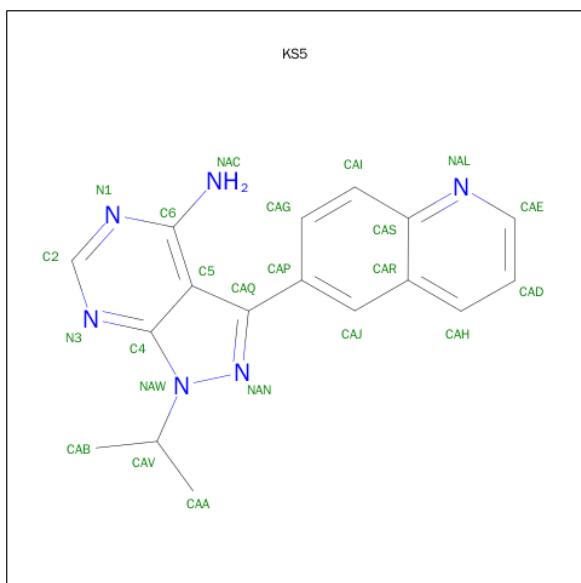
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total 1840	C 1187	N 310	O 328	S 15	0	0	0
1	B	239	Total 1871	C 1200	N 319	O 337	S 15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	EXPRESSION TAG	UNP P00523
A	249	HIS	-	EXPRESSION TAG	UNP P00523
A	250	MET	-	EXPRESSION TAG	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523

- Molecule 2 is 1-(1-METHYLETHYL)-3-QUINOLIN-6-YL-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-AMINE (three-letter code: KS5) (formula: $C_{17}H_{16}N_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 23	C 17	N 6	0	0
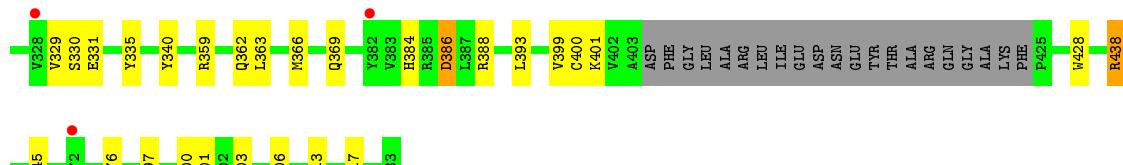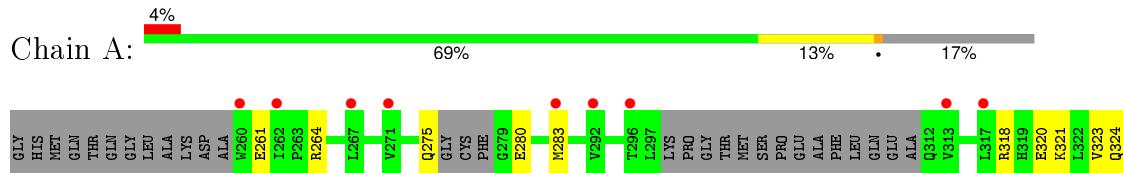
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	9	Total 9	O 9	0	0
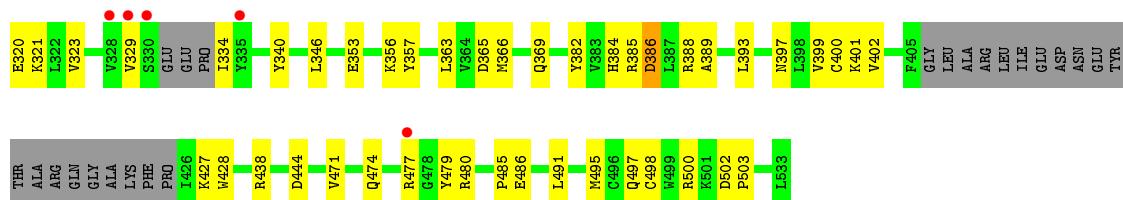
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Proto-oncogene tyrosine-protein kinase Src

• Molecule 1: Proto-oncogene tyrosine-protein kinase Src

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.44Å 63.05Å 74.58Å 101.31° 91.17° 89.62°	Depositor
Resolution (Å)	43.22 – 2.39 43.22 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.2 (43.22-2.39) 90.6 (43.22-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.210 , 0.259 0.206 , 0.253	Depositor DCC
R_{free} test set	1445 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.1	EDS
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 28466 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3749	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: KS5

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	0.77	1/1884 (0.1%)	0.79	1/2558 (0.0%)
1	B	0.74	0/1913	0.82	2/2590 (0.1%)
All	All	0.76	1/3797 (0.0%)	0.81	3/5148 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	CYS	CB-SG	-5.73	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	386	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	444	ASP	CB-CG-OD1	5.68	123.41	118.30

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	1840	0	1787	29	0
1	B	1871	0	1806	39	0

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	16	2	0
3	A	6	0	0	0	0
3	B	9	0	0	1	0
All	All	3749	0	3609	68	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 9.

All (68) 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:384:HIS:HD2	1:B:386:ASP:H	1.12	0.92
1:A:359:ARG:H	1:A:362:GLN:HE21	1.19	0.86
1:B:474:GLN:NE2	1:B:477:ARG:HH11	1.73	0.86
1:A:384:HIS:HD2	1:A:386:ASP:H	1.24	0.85
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.59	0.82
1:B:474:GLN:NE2	1:B:477:ARG:NH1	2.29	0.80
1:A:359:ARG:H	1:A:362:GLN:NE2	1.81	0.79
1:B:474:GLN:HE21	1:B:477:ARG:NH1	1.83	0.74
1:B:264:ARG:HG2	1:B:329:VAL:HG11	1.70	0.74
1:A:320:GLU:O	1:A:401:LYS:HE2	1.89	0.72
1:A:369:GLN:HE22	1:A:399:VAL:HA	1.60	0.67
1:A:323:VAL:HG21	1:A:393:LEU:HD12	1.78	0.64
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.63	0.64
1:B:384:HIS:CD2	1:B:386:ASP:H	2.05	0.63
1:A:359:ARG:HB2	1:A:362:GLN:HE22	1.67	0.60
1:B:369:GLN:HE22	1:B:399:VAL:HA	1.69	0.58
1:A:388:ARG:HB3	1:A:428:TRP:CD1	2.38	0.58
1:B:388:ARG:HG2	1:B:428:TRP:CD1	2.38	0.58
1:A:321:LYS:NZ	1:A:369:GLN:HE21	2.03	0.57
1:B:388:ARG:HG2	1:B:428:TRP:CG	2.40	0.57
1:B:320:GLU:O	1:B:401:LYS:HE2	2.04	0.57
1:B:474:GLN:HE21	1:B:477:ARG:HH11	1.40	0.56
1:B:384:HIS:HD2	1:B:386:ASP:N	1.93	0.56
1:B:363:LEU:HD23	1:B:366:MET:HE3	1.88	0.56
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.42	0.55
1:A:386:ASP:OD2	1:A:388:ARG:NE	2.27	0.54
1:A:318:ARG:HG3	1:A:324:GLN:HE22	1.73	0.53
1:B:264:ARG:HH12	1:B:334:ILE:N	2.07	0.53
1:B:363:LEU:HA	1:B:366:MET:HE3	1.91	0.53
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:VAL:HB	1:A:335:TYR:HB2	1.91	0.52
1:A:476:GLU:HA	1:A:476:GLU:OE2	2.08	0.51
1:B:363:LEU:HD23	1:B:366:MET:CE	2.41	0.51
1:B:321:LYS:NZ	1:B:369:GLN:HE21	2.09	0.50
1:B:283:MET:HG3	1:B:340:TYR:CE1	2.47	0.50
1:A:321:LYS:HA	1:A:401:LYS:HG2	1.94	0.49
1:B:295:LYS:HE2	2:B:2:KS5:CAE	2.42	0.49
1:A:264:ARG:NH1	1:A:331:GLU:O	2.48	0.47
1:B:497:GLN:HE21	1:B:500:ARG:HH22	1.63	0.47
1:B:369:GLN:NE2	1:B:400:CYS:H	2.13	0.46
1:B:384:HIS:O	1:B:385:ARG:HB2	2.15	0.46
1:A:497:GLN:O	1:A:500:ARG:HG3	2.16	0.46
1:B:502:ASP:HA	1:B:503:PRO:HD3	1.73	0.46
1:B:438:ARG:HB3	1:B:438:ARG:HE	1.53	0.45
1:A:321:LYS:HZ2	1:A:369:GLN:HE21	1.64	0.45
1:B:273:LEU:HB2	1:B:281:VAL:O	2.17	0.44
1:B:369:GLN:HE22	1:B:400:CYS:H	1.63	0.44
1:A:321:LYS:NZ	1:A:369:GLN:NE2	2.66	0.44
1:A:261:GLU:OE1	1:A:330:SER:CB	2.65	0.44
1:B:491:LEU:HA	1:B:491:LEU:HD12	1.79	0.43
1:B:365:ASP:C	1:B:365:ASP:OD2	2.57	0.43
1:A:513:GLN:O	1:A:517:GLU:HG3	2.18	0.43
1:A:445:VAL:HG11	1:A:506:ARG:HB3	2.00	0.43
1:B:479:TYR:O	1:B:480:ARG:HD3	2.19	0.43
1:B:317:LEU:HD21	1:B:382:TYR:CD1	2.54	0.42
1:B:497:GLN:NE2	3:B:539:HOH:O	2.53	0.42
1:B:495:MET:O	1:B:498:CYS:HB2	2.20	0.42
1:A:386:ASP:OD1	1:A:388:ARG:NH2	2.52	0.42
1:B:485:PRO:O	1:B:486:GLU:HB2	2.18	0.42
1:A:438:ARG:HH21	1:A:503:PRO:HG2	1.85	0.41
1:B:427:LYS:HE2	1:B:471:VAL:HG21	2.02	0.41
1:A:275:GLN:HE21	1:A:280:GLU:HG2	1.86	0.41
1:B:356:LYS:HE3	1:B:357:TYR:CZ	2.56	0.41
1:A:363:LEU:HA	1:A:366:MET:HE3	2.03	0.41
1:A:362:GLN:O	1:A:366:MET:HG3	2.21	0.41
1:B:321:LYS:NZ	1:B:369:GLN:NE2	2.68	0.40
1:B:273:LEU:HB3	2:B:2:KS5:HAB	2.03	0.40
1:B:346:LEU:HB3	1:B:389:ALA:O	2.21	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	228/286 (80%)	223 (98%)	5 (2%)	0	100	100
1	B	229/286 (80%)	222 (97%)	7 (3%)	0	100	100
All	All	457/572 (80%)	445 (97%)	12 (3%)	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	188/245 (77%)	186 (99%)	2 (1%)	80	92
1	B	190/245 (78%)	184 (97%)	6 (3%)	46	68
All	All	378/490 (77%)	370 (98%)	8 (2%)	61	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	438	ARG
1	A	501	LYS
1	B	290	THR
1	B	316	LYS
1	B	318	ARG
1	B	353	GLU
1	B	397	ASN
1	B	402	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	287	ASN
1	A	324	GLN
1	A	362	GLN
1	A	369	GLN
1	A	384	HIS
1	A	528	GLN
1	B	324	GLN
1	B	369	GLN
1	B	384	HIS
1	B	397	ASN
1	B	474	GLN
1	B	497	GLN
1	B	528	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.

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	KS5	B	2	-	24,26,26	3.17	3 (12%)	27,38,38	3.03	11 (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	KS5	B	2	-	-	0/6/8/8	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	KS5	NAN-NAW	-11.52	1.23	1.37
2	B	2	KS5	CAP-CAQ	-8.87	1.38	1.49
2	B	2	KS5	CAQ-NAN	-3.56	1.32	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	KS5	N3-C2-N1	-8.01	122.76	128.89
2	B	2	KS5	CAG-CAP-CAQ	-4.47	113.51	120.70
2	B	2	KS5	CAA-CAV-NAW	-3.28	107.24	111.46
2	B	2	KS5	CAD-CAE-NAL	-2.83	119.50	123.94
2	B	2	KS5	CAP-CAJ-CAR	-2.38	117.16	121.44
2	B	2	KS5	CAG-CAP-CAJ	2.02	121.19	118.11
2	B	2	KS5	CAH-CAD-CAE	2.09	121.86	118.88
2	B	2	KS5	CAB-CAV-NAW	2.22	114.33	111.46
2	B	2	KS5	CAJ-CAR-CAS	2.80	121.62	118.28
2	B	2	KS5	CAJ-CAP-CAQ	3.14	125.29	120.05
2	B	2	KS5	CAQ-NAN-NAW	9.46	112.13	105.34

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	B	2	KS5	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	236/286 (82%)	0.49	12 (5%)	32	32	17, 27, 38, 49	0
1	B	239/286 (83%)	0.62	19 (7%)	15	15	17, 27, 35, 41	0
All	All	475/572 (83%)	0.56	31 (6%)	22	22	17, 27, 37, 49	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	TYR	5.6
1	A	260	TRP	4.8
1	B	278	PHE	4.7
1	B	282	TRP	4.7
1	B	269	LEU	4.5
1	B	329	VAL	4.0
1	B	296	THR	3.5
1	B	328	VAL	3.4
1	B	283	MET	3.3
1	B	311	ALA	3.1
1	B	285	THR	3.0
1	A	317	LEU	2.7
1	A	296	THR	2.7
1	A	313	VAL	2.6
1	B	286	TRP	2.6
1	A	262	ILE	2.6
1	B	292	VAL	2.6
1	B	294	ILE	2.6
1	A	267	LEU	2.6
1	A	292	VAL	2.5
1	B	271	VAL	2.4
1	A	271	VAL	2.3
1	B	268	ARG	2.3
1	B	330	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	267	LEU	2.3
1	B	272	LYS	2.3
1	A	328	VAL	2.2
1	B	477	ARG	2.1
1	A	472	LEU	2.0
1	A	283	MET	2.0
1	A	382	TYR	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	KS5	B	2	23/23	0.92	0.21	0.98	45,49,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.