



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 02:49 AM EDT

PDB ID : 4FIC / pdb_00004fic
Title : Kinase domain of cSrc in complex with a hinge region-binding fragment
Authors : Richters, A.; Rauh, D.
Deposited on : 2012-06-08
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

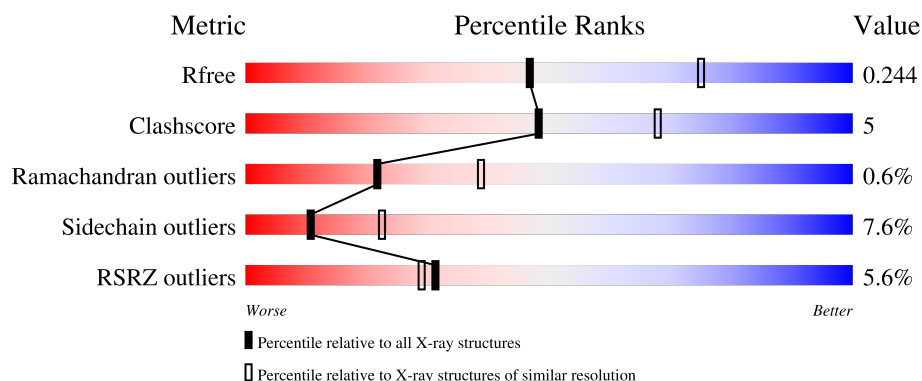
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	286	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	286	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4042 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.

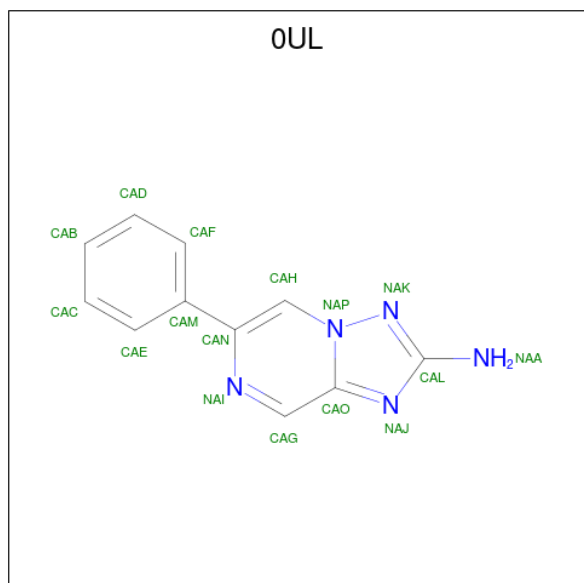
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1975	1271	330	359	15			
1	B	245	Total	C	N	O	S	0	0	0
			1938	1243	327	353	15			

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 6-phenyl[1,2,4]triazolo[1,5-a]pyrazin-2-amine (CCD ID: 0UL) (formula: C₁₁H₉N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			16	11	5		
2	B	1	Total	C	N	0	0
			16	11	5		

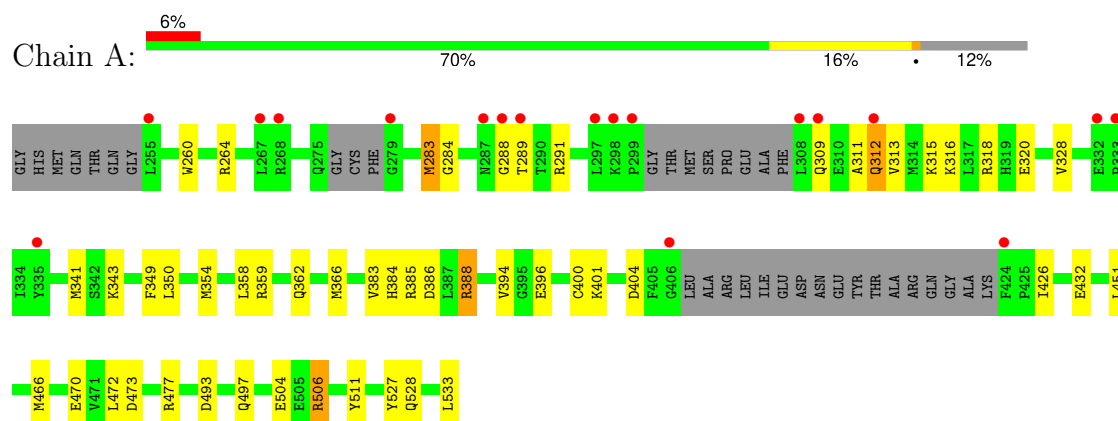
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	48	Total	O	0	0
			48	48		

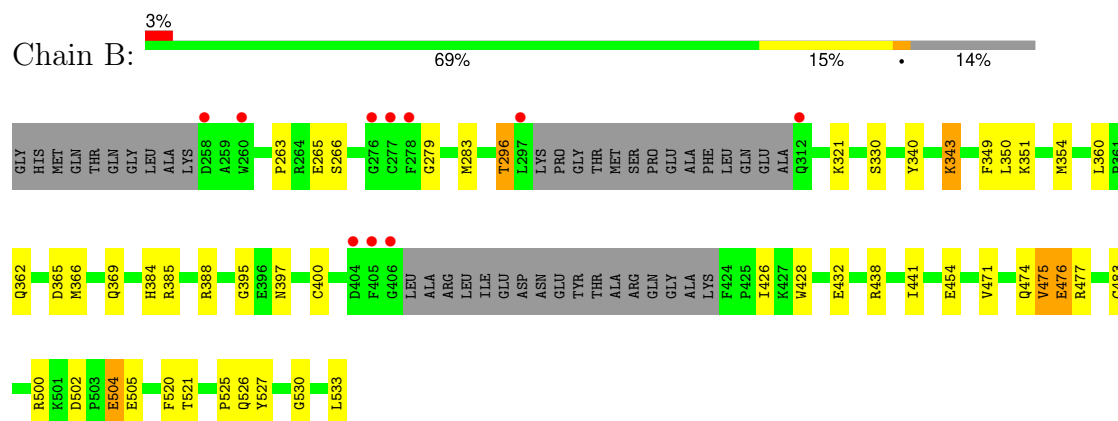
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Proto-oncogene tyrosine-protein kinase Src



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.03Å 63.01Å 73.56Å 79.63° 88.12° 90.17°	Depositor
Resolution (Å)	43.36 – 2.50 43.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.36-2.50) 97.9 (43.36-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.244 0.197 , 0.244	Depositor DCC
R_{free} test set	880 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4042	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% 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: 0UL

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	0.76	0/2022	0.95	3/2743 (0.1%)
1	B	0.77	0/1984	0.98	2/2692 (0.1%)
All	All	0.77	0/4006	0.97	5/5435 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	CYS	CA-C-N	7.39	127.99	120.38
1	B	483	CYS	C-N-CA	7.39	127.99	120.38
1	A	528	GLN	CA-C-N	-6.16	113.44	119.78
1	A	528	GLN	C-N-CA	-6.16	113.44	119.78
1	A	309	GLN	N-CA-C	-5.07	106.19	112.93

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	1975	0	1924	22	0
1	B	1938	0	1893	21	1
2	A	16	0	9	1	0
2	B	16	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	49	0	0	0	0
3	B	48	0	0	1	0
All	All	4042	0	3835	42	1

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 (42) 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:366:MET:HE2	1:B:400:CYS:SG	2.22	0.79
1:B:362:GLN:O	1:B:366:MET:HG3	1.86	0.76
1:B:263:PRO:O	1:B:266:SER:OG	2.13	0.65
1:A:311:ALA:C	1:A:313:VAL:H	2.05	0.64
1:B:471:VAL:O	1:B:475:VAL:HG13	2.00	0.62
1:B:476:GLU:HA	1:B:476:GLU:OE1	2.00	0.60
1:A:341:MET:O	2:A:601:OUL:H9	2.04	0.58
1:A:384:HIS:O	1:A:385:ARG:HB2	2.02	0.58
1:A:283:MET:SD	1:A:291:ARG:HD2	2.45	0.56
1:A:493:ASP:O	1:A:497:GLN:HG3	2.06	0.55
1:A:383:VAL:HG12	1:A:385:ARG:HG3	1.88	0.54
1:B:384:HIS:O	1:B:385:ARG:HB2	2.07	0.54
1:A:386:ASP:OD1	1:A:388:ARG:HD3	2.08	0.54
1:B:527:TYR:OH	1:B:533:LEU:O	2.23	0.52
1:A:511:TYR:HE1	1:B:351:LYS:O	1.92	0.52
1:A:283:MET:HG3	1:A:284:GLY:N	2.26	0.50
1:B:428:TRP:HE1	1:B:454:GLU:CD	2.20	0.50
1:A:362:GLN:O	1:A:366:MET:HG3	2.12	0.49
1:B:343:LYS:HG3	1:B:395:GLY:O	2.13	0.49
1:A:311:ALA:C	1:A:313:VAL:N	2.67	0.49
1:A:320:GLU:O	1:A:401:LYS:HE2	2.13	0.48
1:B:504:GLU:H	1:B:504:GLU:CD	2.22	0.47
1:B:366:MET:CE	1:B:400:CYS:SG	3.00	0.46
1:A:312:GLN:O	1:A:316:LYS:HG3	2.16	0.46
1:B:321:LYS:HD2	1:B:369:GLN:HB3	1.98	0.45
1:B:349:PHE:CE1	1:B:354:MET:HG3	2.53	0.44
1:B:474:GLN:OE1	1:B:477:ARG:NH1	2.46	0.43
1:B:520:PHE:O	1:B:525:PRO:HA	2.19	0.42
1:B:283:MET:HG3	1:B:340:TYR:CE1	2.55	0.41
1:A:366:MET:HE2	1:A:400:CYS:SG	2.60	0.41
1:A:260:TRP:CD1	1:A:315:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:MET:HE3	1:A:470:GLU:HG2	2.03	0.41
1:A:527:TYR:OH	1:A:533:LEU:O	2.33	0.41
1:B:530:GLY:HA3	3:B:738:HOH:O	2.19	0.41
1:A:343:LYS:HB2	1:A:394:VAL:HB	2.03	0.41
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.54	0.41
1:A:358:LEU:O	1:A:359:ARG:NH1	2.52	0.41
1:B:279:GLY:HA3	1:B:296:THR:O	2.21	0.41
1:A:349:PHE:CE1	1:A:354:MET:HG3	2.56	0.41
1:B:384:HIS:O	1:B:385:ARG:CB	2.69	0.41
1:A:432:GLU:OE1	1:A:506:ARG:NH2	2.54	0.40
1:A:473:ASP:O	1:A:477:ARG:HG3	2.21	0.40

All (1) 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)
1:B:397:ASN:OD1	1:B:438:ARG:NE[1_455]	2.13	0.07

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	243/286 (85%)	230 (95%)	10 (4%)	3 (1%)	11	21
1	B	239/286 (84%)	224 (94%)	15 (6%)	0	100	100
All	All	482/572 (84%)	454 (94%)	25 (5%)	3 (1%)	22	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	GLY
1	A	264	ARG

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Mol	Chain	Res	Type
1	A	312	GLN

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	205/245 (84%)	192 (94%)	13 (6%)	15	30
1	B	203/245 (83%)	185 (91%)	18 (9%)	8	17
All	All	408/490 (83%)	377 (92%)	31 (8%)	11	22

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	MET
1	A	289	THR
1	A	318	ARG
1	A	328	VAL
1	A	350	LEU
1	A	388	ARG
1	A	396	GLU
1	A	404	ASP
1	A	426	ILE
1	A	451	LEU
1	A	472	LEU
1	A	504	GLU
1	A	506	ARG
1	B	265	GLU
1	B	296	THR
1	B	330	SER
1	B	343	LYS
1	B	350	LEU
1	B	360	LEU
1	B	365	ASP
1	B	426	ILE
1	B	432	GLU

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Mol	Chain	Res	Type
1	B	441	ILE
1	B	475	VAL
1	B	476	GLU
1	B	500	ARG
1	B	502	ASP
1	B	504	GLU
1	B	505	GLU
1	B	521	THR
1	B	526	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	497	GLN
1	A	526	GLN
1	A	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0UL	A	601	-	14,18,18	2.62	3 (21%)	14,25,25	1.70	3 (21%)
2	0UL	B	601	-	14,18,18	2.65	3 (21%)	14,25,25	1.91	2 (14%)

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	0UL	A	601	-	-	0/4/4/4	0/3/3/3
2	0UL	B	601	-	-	0/4/4/4	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	0UL	CAG-CAO	-6.59	1.34	1.41
2	A	601	0UL	CAG-CAO	-6.27	1.34	1.41
2	B	601	0UL	CAG-NAI	5.55	1.42	1.32
2	A	601	0UL	CAM-CAN	-5.39	1.40	1.49
2	A	601	0UL	CAG-NAI	4.76	1.41	1.32
2	B	601	0UL	CAM-CAN	-4.47	1.42	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	0UL	CAG-NAI-CAN	6.06	122.23	117.55
2	A	601	0UL	CAG-NAI-CAN	5.03	121.43	117.55
2	B	601	0UL	CAM-CAN-NAI	2.24	121.03	116.87
2	A	601	0UL	CAM-CAN-NAI	2.21	120.97	116.87
2	A	601	0UL	CAH-CAN-CAM	-2.04	119.95	122.13

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	0UL	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	251/286 (87%)	0.10	18 (7%) 23 21	19, 36, 82, 99	0
1	B	245/286 (85%)	-0.03	10 (4%) 42 39	16, 36, 75, 105	0
All	All	496/572 (86%)	0.04	28 (5%) 31 29	16, 36, 80, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	CYS	4.8
1	B	297	LEU	4.3
1	A	406	GLY	4.1
1	A	255	LEU	4.0
1	A	299	PRO	3.7
1	B	406	GLY	3.5
1	B	278	PHE	3.5
1	A	424	PHE	3.4
1	A	279	GLY	3.3
1	A	287	ASN	3.2
1	A	335	TYR	3.2
1	B	260	TRP	3.2
1	B	276	GLY	3.1
1	A	309	GLN	3.1
1	B	312	GLN	2.9
1	A	289	THR	2.9
1	A	332	GLU	2.9
1	B	404	ASP	2.8
1	A	312	GLN	2.7
1	B	405	PHE	2.6
1	A	333	PRO	2.6
1	A	297	LEU	2.4
1	A	267	LEU	2.4
1	B	258	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	LYS	2.3
1	A	268	ARG	2.1
1	A	308	LEU	2.1
1	A	288	GLY	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 monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
2	0UL	A	601	16/16	0.92	0.11	44,48,54,55	0
2	0UL	B	601	16/16	0.92	0.10	37,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.