Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:26 AM GMT

PDB ID	:	2QQ7
Title	:	Crystal structure of drug resistant SRC kinase domain with irreversible inhibitor
Authors	:	Michalczyk, A.; Rode, H.B.; Gruetter, C.; Rauh, D.
Deposited on	:	2007-07-26
Resolution	:	2.38 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

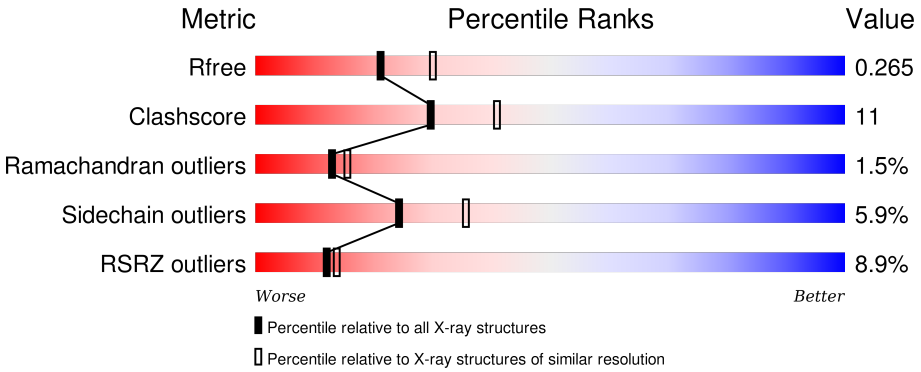
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	10% 67% 18% • • 12%
1	B	286	5% 70% 13% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4160 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.

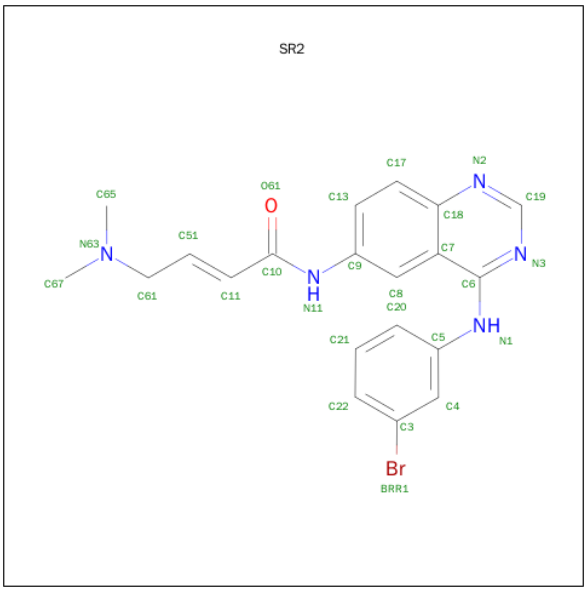
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	1	2	0
			1988	1278	334	359	17			
1	B	244	Total	C	N	O	S	0	0	0
			1950	1252	326	355	17			

There are 10 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
A	338	MET	THR	ENGINEERED	UNP P00523
A	345	CYS	SER	ENGINEERED	UNP P00523
B	248	GLY	-	EXPRESSION TAG	UNP P00523
B	249	HIS	-	EXPRESSION TAG	UNP P00523
B	250	MET	-	EXPRESSION TAG	UNP P00523
B	338	MET	THR	ENGINEERED	UNP P00523
B	345	CYS	SER	ENGINEERED	UNP P00523

- Molecule 2 is (2E)-N-{4-[(3-BROMOPHENYL)AMINO]QUINAZOLIN-6-YL}-4-(DIMETHYLAMINO)BUT-2-ENAMIDE (three-letter code: SR2) (formula: $C_{20}H_{20}BrN_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			27	1	20	5	1		
2	B	1	Total	Br	C	N	O	0	0
			27	1	20	5	1		

- Molecule 3 is water.

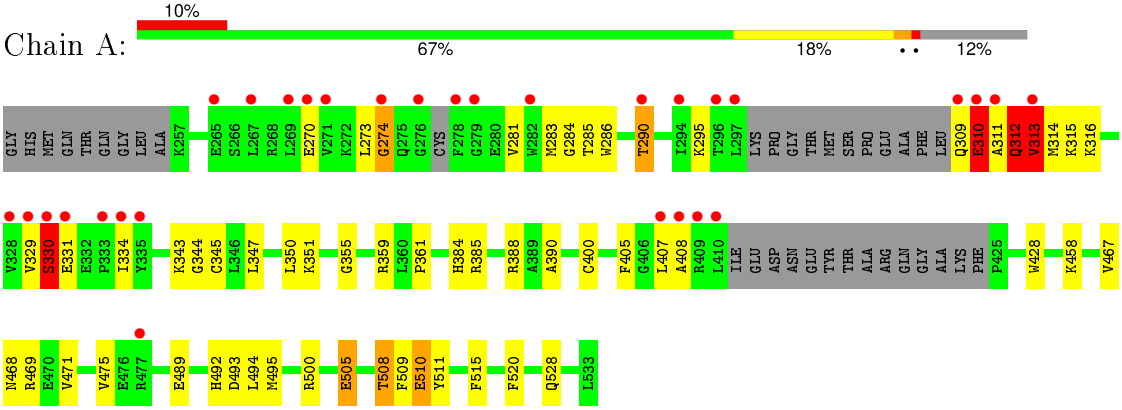
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		
3	B	75	Total	O	0	0
			75	75		

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.

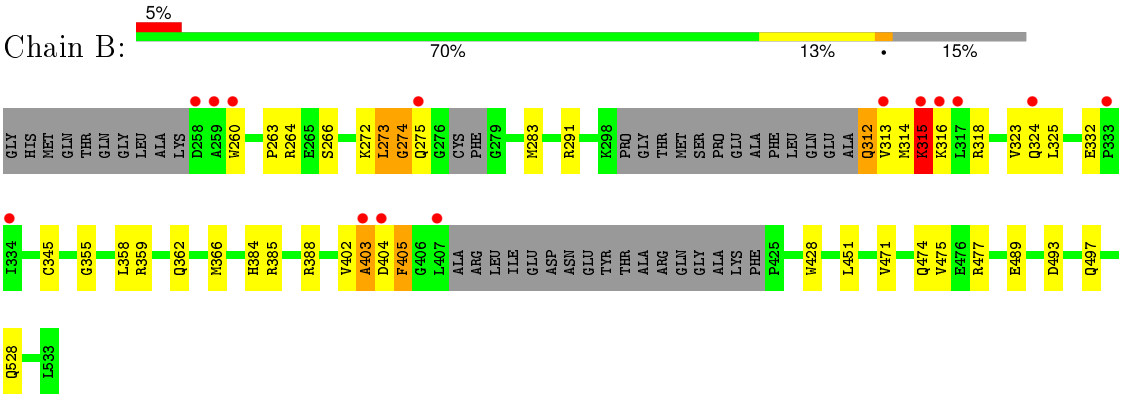
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.22Å 63.36Å 75.06Å 78.58° 89.08° 89.87°	Depositor
Resolution (Å)	73.52 – 2.38 43.41 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (73.52-2.38) 91.8 (43.41-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	13.44 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.266 0.215 , 0.265	Depositor DCC
R_{free} test set	1518 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.1	EDS
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 29935 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4160	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 7.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SR2

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	0.85	1/2040 (0.0%)	0.80	1/2762 (0.0%)
1	B	0.78	0/1995	0.80	0/2699
All	All	0.82	1/4035 (0.0%)	0.80	1/5461 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	5
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	400	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	VAL	CB-CA-C	5.13	121.14	111.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	312	GLN	Peptide
1	A	330	SER	Peptide
1	B	273	LEU	Peptide
1	B	315	LYS	Peptide
1	B	316	LYS	Peptide
1	B	402	VAL	Peptide
1	B	403	ALA	Peptide

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	1988	0	1937	53	0
1	B	1950	0	1921	34	0
2	A	27	0	19	5	0
2	B	27	0	19	2	0
3	A	93	0	0	0	0
3	B	75	0	0	0	0
All	All	4160	0	3896	88	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 11.

All (88) 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:404:ASP:N	1:B:405:PHE:HA	1.45	1.25
1:B:403:ALA:HB1	1:B:404:ASP:HA	1.21	1.20
1:B:404:ASP:H	1:B:405:PHE:CA	1.56	1.19
1:A:312:GLN:HB3	1:A:313:VAL:HG23	1.32	1.12
1:B:403:ALA:CB	1:B:404:ASP:HA	1.97	0.94
1:B:315:LYS:N	1:B:315:LYS:HD2	1.80	0.93
1:A:508:THR:HG21	1:A:510:GLU:HG2	1.49	0.93
1:A:355:GLY:O	1:A:458:LYS:HE2	1.72	0.90
1:A:330:SER:CB	1:A:331:GLU:HB2	2.05	0.86
1:A:508:THR:CG2	1:A:510:GLU:H	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ASP:N	1:B:405:PHE:CA	2.26	0.85
1:B:404:ASP:H	1:B:405:PHE:HA	0.71	0.84
1:A:311:ALA:O	1:A:312:GLN:HB2	1.75	0.83
1:A:309:GLN:O	1:A:313:VAL:HG21	1.79	0.81
1:B:358:LEU:O	1:B:359:ARG:NH1	2.14	0.80
1:A:508:THR:HG22	1:A:510:GLU:N	1.96	0.80
1:A:295:LYS:HB2	2:A:1345:SR2:BRR1	2.39	0.77
1:A:309:GLN:O	1:A:313:VAL:CG2	2.34	0.76
1:B:403:ALA:HB1	1:B:404:ASP:CA	2.11	0.76
1:B:313:VAL:H	1:B:314:MET:HB2	1.56	0.71
1:A:508:THR:HG21	1:A:510:GLU:CG	2.20	0.69
1:A:312:GLN:CB	1:A:313:VAL:HG23	2.18	0.69
1:A:345:CYS:SG	2:A:1345:SR2:H673	2.34	0.67
1:A:508:THR:CG2	1:A:510:GLU:N	2.57	0.67
1:B:272:LYS:HG2	1:B:274:GLY:HA2	1.77	0.66
1:A:385:ARG:HD2	1:A:407:LEU:O	1.95	0.66
1:A:508:THR:HG22	1:A:510:GLU:H	1.57	0.66
1:A:329:VAL:O	1:A:331:GLU:N	2.29	0.65
1:B:260:TRP:CD2	1:B:315:LYS:HE2	2.32	0.64
1:B:315:LYS:H	1:B:315:LYS:HD2	1.62	0.63
1:B:315:LYS:HG3	1:B:325:LEU:HD23	1.82	0.62
1:A:345:CYS:HB3	2:A:1345:SR2:O61	2.00	0.62
1:B:312:GLN:N	1:B:314:MET:O	2.35	0.60
1:A:283:MET:HG3	1:A:284:GLY:N	2.16	0.60
1:A:508:THR:HG23	1:A:510:GLU:H	1.65	0.60
1:B:273:LEU:H	1:B:274:GLY:HA2	1.66	0.60
1:A:273:LEU:H	1:A:274:GLY:HA3	1.68	0.59
1:B:263:PRO:O	1:B:266:SER:OG	2.20	0.58
1:B:345:CYS:HB3	2:B:1345:SR2:O61	2.04	0.58
1:A:286:TRP:HB3	1:A:290:THR:HB	1.86	0.57
1:B:403:ALA:CB	1:B:404:ASP:CA	2.76	0.56
1:B:474:GLN:OE1	1:B:477:ARG:NH1	2.38	0.56
1:A:508:THR:HG22	1:A:511:TYR:H	1.70	0.56
1:A:329:VAL:O	1:A:330:SER:C	2.46	0.54
1:B:264:ARG:HH22	1:B:332:GLU:H	1.56	0.54
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.90	0.54
1:B:260:TRP:CZ2	1:B:315:LYS:HG2	2.44	0.53
1:B:384:HIS:NE2	1:B:403:ALA:O	2.33	0.52
1:B:405:PHE:CD1	1:B:405:PHE:N	2.78	0.52
1:A:310:GLU:O	1:A:313:VAL:HB	2.08	0.51
1:A:344:GLY:HA2	2:A:1345:SR2:C13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:HIS:O	1:A:385:ARG:HB2	2.12	0.50
1:A:388[A]:ARG:NH1	1:A:390:ALA:HB3	2.26	0.50
1:B:362:GLN:O	1:B:366:MET:HG3	2.12	0.49
1:A:311:ALA:O	1:A:312:GLN:CB	2.54	0.49
1:A:508:THR:CG2	1:A:509:PHE:N	2.74	0.49
1:A:283:MET:HG3	1:A:284:GLY:H	1.79	0.48
1:B:264:ARG:NH2	1:B:332:GLU:H	2.11	0.48
2:B:1345:SR2:H4	2:B:1345:SR2:N3	2.29	0.47
1:A:345:CYS:SG	2:A:1345:SR2:C67	3.01	0.47
1:A:285:THR:HG22	1:A:286:TRP:H	1.80	0.46
1:B:388:ARG:HB3	1:B:428:TRP:CD1	2.51	0.46
1:B:471:VAL:O	1:B:475:VAL:HG23	2.16	0.46
1:A:330:SER:O	1:A:334:ILE:HG12	2.16	0.45
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.52	0.45
1:B:384:HIS:O	1:B:385:ARG:HB2	2.16	0.45
1:A:508:THR:CG2	1:A:510:GLU:CG	2.93	0.45
1:A:273:LEU:N	1:A:274:GLY:HA3	2.32	0.45
1:B:315:LYS:HB2	1:B:318:ARG:NH2	2.32	0.44
1:A:508:THR:HG23	1:A:509:PHE:N	2.33	0.44
1:B:493:ASP:O	1:B:497:GLN:HG3	2.18	0.44
1:A:274:GLY:HA2	1:A:281:VAL:HB	1.99	0.43
1:A:388[A]:ARG:HB3	1:A:428:TRP:CD1	2.53	0.43
1:A:313:VAL:O	1:A:315:LYS:N	2.52	0.43
1:B:260:TRP:CG	1:B:315:LYS:HE2	2.54	0.42
1:B:283:MET:SD	1:B:291:ARG:NH1	2.93	0.42
1:A:330:SER:CB	1:A:331:GLU:CB	2.89	0.42
1:A:385:ARG:CD	1:A:407:LEU:O	2.65	0.42
1:A:494:LEU:HD22	1:A:515:PHE:CE1	2.55	0.42
1:A:510:GLU:HG3	1:A:511:TYR:N	2.34	0.41
1:A:467:VAL:HG12	1:A:468:ASN:H	1.85	0.41
1:A:492:HIS:O	1:A:495:MET:HB2	2.20	0.41
1:A:350:LEU:O	1:A:355:GLY:HA3	2.20	0.41
1:B:315:LYS:N	1:B:315:LYS:CD	2.64	0.41
1:A:471:VAL:O	1:A:475:VAL:HG23	2.20	0.41
1:A:405:PHE:HD2	1:A:408:ALA:CB	2.33	0.41
1:A:343:LYS:HD3	1:A:343:LYS:HA	1.85	0.41
1:A:329:VAL:HG12	1:A:331:GLU:HB3	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	245/286 (86%)	229 (94%)	11 (4%)	5 (2%)	9 10
1	B	236/286 (82%)	219 (93%)	15 (6%)	2 (1%)	24 33
All	All	481/572 (84%)	448 (93%)	26 (5%)	7 (2%)	13 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	B	355	GLY
1	A	313	VAL
1	A	330	SER
1	A	274	GLY
1	A	314	MET
1	B	274	GLY

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%)	189 (92%)	16 (8%)	16 22
1	B	207/245 (84%)	198 (96%)	9 (4%)	35 52
All	All	412/490 (84%)	387 (94%)	25 (6%)	24 34

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

Mol	Chain	Res	Type
1	A	270	GLU
1	A	290	THR
1	A	310	GLU
1	A	313	VAL
1	A	316	LYS
1	A	347	LEU
1	A	351	LYS
1	A	359	ARG
1	A	469	ARG
1	A	489	GLU
1	A	493[A]	ASP
1	A	493[B]	ASP
1	A	505	GLU
1	A	508	THR
1	A	510	GLU
1	A	528	GLN
1	B	275	GLN
1	B	312	GLN
1	B	315	LYS
1	B	323	VAL
1	B	324	GLN
1	B	405	PHE
1	B	451	LEU
1	B	489	GLU
1	B	528	GLN

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)

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	SR2	A	1345	1	29,29,29	2.28	6 (20%)	37,39,39	3.24	11 (29%)
2	SR2	B	1345	1	29,29,29	2.47	6 (20%)	37,39,39	3.04	11 (29%)

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	SR2	A	1345	1	-	1/14/14/14	0/3/3/3
2	SR2	B	1345	1	-	1/14/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1345	SR2	C6-C7	-3.91	1.40	1.44
2	A	1345	SR2	C9-N11	-3.66	1.34	1.41
2	A	1345	SR2	C5-N1	-3.43	1.33	1.40
2	B	1345	SR2	C9-N11	-3.43	1.35	1.41
2	B	1345	SR2	C6-C7	-2.93	1.41	1.44
2	B	1345	SR2	C5-N1	-2.61	1.35	1.40
2	A	1345	SR2	C61-C51	2.22	1.55	1.49
2	B	1345	SR2	C61-C51	2.54	1.56	1.49
2	A	1345	SR2	C11-C10	3.00	1.54	1.48
2	B	1345	SR2	C11-C10	3.80	1.55	1.48
2	A	1345	SR2	C11-C51	8.77	1.56	1.31
2	B	1345	SR2	C11-C51	10.38	1.60	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1345	SR2	N2-C19-N3	-10.60	120.78	128.89
2	B	1345	SR2	N2-C19-N3	-10.00	121.24	128.89
2	A	1345	SR2	C61-C51-C11	-8.17	113.11	124.76
2	B	1345	SR2	C61-C51-C11	-7.18	114.53	124.76
2	A	1345	SR2	C8-C7-C6	-6.34	121.51	124.89
2	B	1345	SR2	C7-C6-N3	-4.44	118.29	121.46
2	B	1345	SR2	C8-C7-C6	-3.86	122.83	124.89
2	A	1345	SR2	C7-C6-N3	-3.60	118.89	121.46
2	B	1345	SR2	C9-N11-C10	-3.59	123.12	128.37
2	B	1345	SR2	C7-C18-N2	-2.75	119.96	122.88
2	A	1345	SR2	C9-N11-C10	-2.36	124.91	128.37
2	A	1345	SR2	C7-C18-N2	-2.13	120.62	122.88
2	A	1345	SR2	O61-C10-N11	2.05	125.54	122.95
2	B	1345	SR2	C5-C4-C3	2.52	121.29	118.74
2	A	1345	SR2	C6-C7-C18	2.65	117.28	115.77
2	B	1345	SR2	N1-C6-N3	2.68	121.39	118.85
2	A	1345	SR2	N1-C6-N3	3.87	122.52	118.85
2	B	1345	SR2	C6-C7-C18	4.02	118.06	115.77
2	A	1345	SR2	C19-N2-C18	5.87	120.61	115.19
2	B	1345	SR2	C19-N2-C18	6.12	120.84	115.19
2	B	1345	SR2	C19-N3-C6	7.11	121.60	116.48
2	A	1345	SR2	C19-N3-C6	7.41	121.81	116.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1345	SR2	C10-C11-C51-C61
2	A	1345	SR2	C10-C11-C51-C61

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1345	SR2	5	0
2	B	1345	SR2	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, 95^{th} 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%)	0.67	30 (11%) 6 7	12, 29, 65, 76	2 (0%)
1	B	244/286 (85%)	0.56	14 (5%) 27 31	13, 30, 59, 73	3 (1%)
All	All	495/572 (86%)	0.61	44 (8%) 12 14	12, 30, 64, 76	5 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	404	ASP	7.0
1	B	313	VAL	5.1
1	A	269	LEU	5.1
1	A	331	GLU	4.8
1	A	335	TYR	4.6
1	A	267	LEU	4.6
1	A	276	GLY	4.4
1	B	260	TRP	4.3
1	A	330	SER	4.3
1	A	278	PHE	4.3
1	A	334	ILE	4.1
1	A	408	ALA	4.0
1	B	316	LYS	3.8
1	B	259	ALA	3.7
1	B	333	PRO	3.7
1	B	324	GLN	3.6
1	A	409	ARG	3.6
1	A	270	GLU	3.5
1	A	311	ALA	3.2
1	A	282	TRP	3.2
1	B	315	LYS	3.1
1	A	328	VAL	3.0
1	A	329	VAL	2.9
1	B	334	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	297	LEU	2.9
1	A	310	GLU	2.8
1	A	333	PRO	2.8
1	A	271	VAL	2.8
1	B	403	ALA	2.8
1	A	313	VAL	2.7
1	A	274	GLY	2.7
1	A	407	LEU	2.5
1	B	407	LEU	2.5
1	B	258	ASP	2.5
1	B	275	GLN	2.4
1	A	309	GLN	2.4
1	A	294	ILE	2.3
1	A	410	LEU	2.3
1	B	317	LEU	2.3
1	A	290	THR	2.3
1	A	279	GLY	2.3
1	A	296	THR	2.2
1	A	265	GLU	2.1
1	A	477	ARG	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, 95^{th} 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	SR2	A	1345	27/27	0.81	0.22	0.82	45,66,76,79	0
2	SR2	B	1345	27/27	0.80	0.26	0.73	45,60,73,76	0

6.5 Other polymers (i)

There are no such residues in this entry.