Full wwPDB X-ray Structure Validation Report (i)

Jul 5, 2022 – 02:51 PM JST

PDB ID	:	7Y8S
Title	:	Crystal structure of sDscam FNIII1-3 domains, isoform beta2v6
Deposited on	:	2022-06-24
Resolution	:	2.70 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

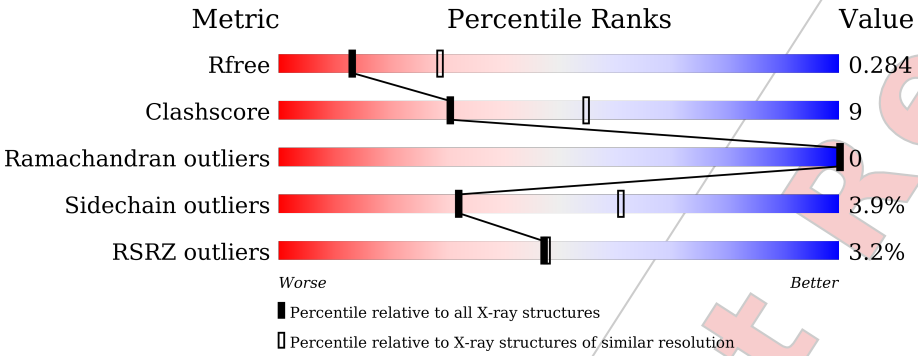
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1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	298	3% 69% 21% 8%
1	B	298	3% 77% 20%

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2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8827 atoms, of which 4319 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 Dscam.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	H	N	O	S	2	0	0
			4290	1389	2122	364	412	3			
1	B	288	Total	C	H	N	O	S	0	0	0
			4464	1449	2197	380	435	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	GLY	-	expression tag	UNP A0A161FW14
A	293	ALA	-	expression tag	UNP A0A161FW14
A	294	SER	-	expression tag	UNP A0A161FW14
B	292	GLY	-	expression tag	UNP A0A161FW14
B	293	ALA	-	expression tag	UNP A0A161FW14
B	294	SER	-	expression tag	UNP A0A161FW14

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	2	Total	Na	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	42	Total	O	0	0
			42	42		

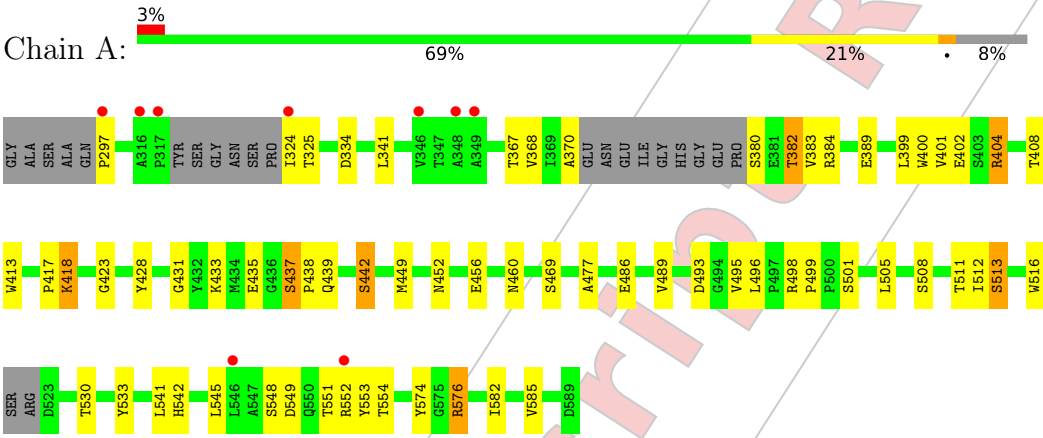
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3 Residue-property plots (i)

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.

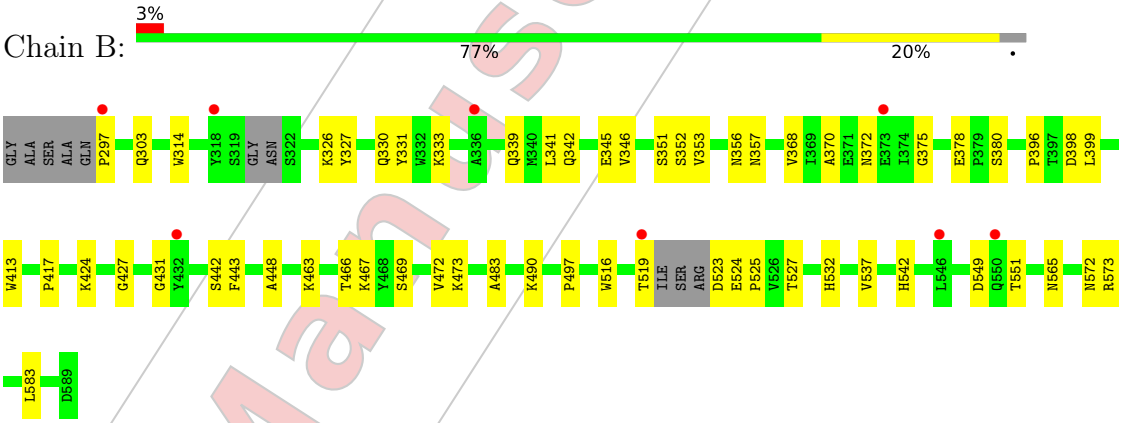
• Molecule 1: Dscam

Chain A:



• Molecule 1: Dscam

Chain B:



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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	171.65Å 171.65Å 114.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.20 – 2.70 40.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	89.2 (40.20-2.70) 89.3 (40.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.226 , 0.284 0.226 , 0.284	Depositor DCC
R_{free} test set	1260 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8827	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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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: NA

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	0.33	0/2227	0.58	0/3037
1	B	0.30	0/2331	0.54	0/3181
All	All	0.31	0/4558	0.56	0/6218

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	THR	Peptide
1	A	437	SER	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	2122	2137	48	0
1	B	2267	2197	2219	37	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	28	0	0	4	0
3	B	42	0	0	2	0
All	All	4508	4319	4356	81	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 (81) 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:530:THR:OG1	1:A:576:ARG:NH1	1.79	1.12
1:A:368:VAL:O	1:A:380:SER:OG	1.89	0.90
1:B:524:GLU:OE1	1:B:573:ARG:NH1	2.06	0.88
1:A:530:THR:CB	1:A:576:ARG:HH11	1.98	0.76
1:A:496:LEU:O	3:A:701:HOH:O	2.05	0.74
1:A:417:PRO:HG2	1:B:417:PRO:HG2	1.75	0.69
1:A:412:ARG:NH2	1:A:456:GLU:OE1	2.26	0.68
1:B:497:PRO:O	3:B:701:HOH:O	2.11	0.68
1:A:542:HIS:NE2	3:A:706:HOH:O	2.27	0.67
1:B:537:VAL:O	1:B:537:VAL:HG23	1.98	0.63
1:A:513:SER:HG	1:A:554:THR:HG1	1.42	0.62
1:B:467:LYS:HG3	1:B:490:LYS:HG3	1.83	0.61
1:A:508:SER:OG	1:A:511:THR:N	2.33	0.60
1:B:356:ASN:O	3:B:702:HOH:O	2.16	0.60
1:A:428:TYR:OH	3:A:702:HOH:O	2.16	0.60
1:A:399:LEU:HD23	1:A:413:TRP:HB3	1.85	0.59
1:B:524:GLU:HB3	1:B:525:PRO:HD2	1.85	0.58
1:B:519:THR:O	1:B:523:ASP:OD1	2.22	0.58
1:A:431:GLY:HA2	1:A:442:SER:O	2.05	0.56
1:A:389:GLU:HG3	1:A:423:GLY:HA3	1.88	0.56
1:B:516:TRP:O	1:B:551:THR:OG1	2.24	0.56
1:A:493:ASP:HB3	1:A:495:VAL:H	1.71	0.55
1:B:297:PRO:HG3	1:B:370:ALA:HB2	1.89	0.54
1:A:418:LYS:NZ	3:A:704:HOH:O	2.23	0.54
1:A:367:THR:OG1	1:A:382:THR:HB	2.09	0.52
1:A:486:GLU:O	1:B:357:ASN:ND2	2.39	0.52
1:A:324:ILE:HG22	1:A:325:THR:H	1.74	0.52
1:B:519:THR:O	1:B:519:THR:OG1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HD11	1:A:553:TYR:CE1	2.46	0.51
1:B:537:VAL:O	1:B:537:VAL:CG2	2.57	0.51
1:B:463:LYS:N	1:B:463:LYS:HD2	2.25	0.51
1:A:404:ARG:HB2	1:A:408:THR:OG1	2.11	0.51
1:B:314:TRP:O	1:B:351:SER:OG	2.29	0.50
1:B:463:LYS:HB2	1:B:466:THR:HG21	1.94	0.50
1:B:297:PRO:HD2	1:B:368:VAL:CG1	2.42	0.49
1:A:417:PRO:CG	1:B:417:PRO:HG2	2.42	0.49
1:A:505:LEU:HD11	1:A:552:ARG:HG2	1.95	0.49
1:B:326:LYS:NZ	1:B:345:GLU:HG2	2.28	0.49
1:B:527:THR:HG23	1:B:572:ASN:HA	1.95	0.48
1:A:408:THR:HG22	1:A:460:ASN:CB	2.44	0.48
1:B:331:TYR:CE1	1:B:342:GLN:HG3	2.50	0.47
1:A:297:PRO:HG3	1:A:368:VAL:O	2.15	0.47
1:A:409:ILE:HD13	1:A:489:VAL:CG1	2.45	0.46
1:A:512:ILE:HD13	1:A:585:VAL:HG13	1.98	0.46
1:B:333:LYS:HB2	1:B:339:GLN:HE21	1.80	0.46
1:B:427:GLY:HA2	1:B:448:ALA:N	2.31	0.45
1:B:327:TYR:HB2	1:B:346:VAL:HG13	1.97	0.45
1:B:565:ASN:HA	1:B:583:LEU:O	2.16	0.45
1:A:582:ILE:O	1:A:582:ILE:CG2	2.65	0.45
1:B:532:HIS:ND1	1:B:542:HIS:CE1	2.85	0.45
1:A:411:VAL:O	1:A:456:GLU:HA	2.16	0.44
1:A:334:ASP:OD2	1:A:384:ARG:HD3	2.18	0.44
1:A:401:VAL:HG12	1:A:411:VAL:HG13	1.98	0.44
1:A:437:SER:HB3	1:A:438:PRO:HD3	2.00	0.44
1:A:324:ILE:HD12	1:A:324:ILE:N	2.33	0.43
1:B:473:LYS:HG2	1:B:483:ALA:HA	2.01	0.43
1:A:400:TRP:CH2	1:A:402:GLU:HG3	2.53	0.43
1:A:582:ILE:HG22	1:B:339:GLN:HB2	2.01	0.43
1:B:396:PRO:HG2	1:B:472:VAL:HG12	2.00	0.43
1:A:449:MET:HB3	1:A:452:ASN:OD1	2.18	0.43
1:B:297:PRO:HG3	1:B:327:TYR:CE2	2.53	0.42
1:B:314:TRP:CH2	1:B:353:VAL:HG23	2.54	0.42
1:B:372:ASN:HB3	1:B:375:GLY:H	1.84	0.42
1:A:498:ARG:HB2	1:A:499:PRO:HD2	2.01	0.42
1:A:382:THR:HG1	1:A:383:VAL:H	1.67	0.42
1:A:324:ILE:HG22	1:A:325:THR:N	2.34	0.42
1:A:516:TRP:O	1:A:551:THR:HB	2.19	0.42
1:B:330:GLN:HB3	1:B:341:LEU:HD11	2.02	0.42
1:A:324:ILE:HG21	1:A:370:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:HG3	1:A:380:SER:HG	1.85	0.42
1:A:495:VAL:HG12	1:A:574:TYR:CG	2.55	0.42
1:A:469:SER:OG	1:A:486:GLU:HG2	2.20	0.41
1:B:399:LEU:HD23	1:B:413:TRP:HB3	2.03	0.41
1:B:431:GLY:HA3	1:B:443:PHE:CE1	2.56	0.41
1:A:400:TRP:CH2	1:A:402:GLU:HB2	2.56	0.41
1:A:433:LYS:HE3	1:A:439:GLN:O	2.21	0.41
1:A:533:TYR:CE2	1:A:541:LEU:HD12	2.56	0.41
1:B:524:GLU:OE1	1:B:525:PRO:HD2	2.21	0.41
1:B:378:GLU:H	1:B:378:GLU:HG2	1.69	0.40
1:A:408:THR:HG22	1:A:460:ASN:HA	2.03	0.40
1:A:389:GLU:OE1	1:A:477:ALA:N	2.51	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	267/298 (90%)	254 (95%)	13 (5%)	0	100	100
1	B	282/298 (95%)	276 (98%)	6 (2%)	0	100	100
All	All	549/596 (92%)	530 (96%)	19 (4%)	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

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analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/256 (93%)	228 (95%)	11 (5%)	27	54
1	B	250/256 (98%)	242 (97%)	8 (3%)	39	68
All	All	489/512 (96%)	470 (96%)	19 (4%)	32	61

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	LEU
1	A	404	ARG
1	A	418	LYS
1	A	435	GLU
1	A	442	SER
1	A	501	SER
1	A	513	SER
1	A	518	HIS
1	A	548	SER
1	A	549	ASP
1	A	576	ARG
1	B	303	GLN
1	B	352	SER
1	B	380	SER
1	B	398	ASP
1	B	424	LYS
1	B	442	SER
1	B	469	SER
1	B	549	ASP

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	422	HIS
1	A	518	HIS
1	B	339	GLN
1	B	350	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

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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	275/298 (92%)	0.00	10 (3%) 42 42	19, 40, 79, 96	1 (0%)
1	B	288/298 (96%)	-0.03	8 (2%) 53 54	19, 38, 74, 115	0
All	All	563/596 (94%)	-0.01	18 (3%) 47 48	19, 38, 76, 115	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	546	LEU	8.2
1	B	297	PRO	7.7
1	A	317	PRO	6.1
1	A	297	PRO	5.3
1	B	519	THR	3.8
1	A	324	ILE	3.5
1	A	518	HIS	2.9
1	A	316	ALA	2.5
1	A	349	ALA	2.3
1	A	346	VAL	2.3
1	A	552	ARG	2.2
1	B	432	TYR	2.2
1	B	550	GLN	2.2
1	B	318	TYR	2.1
1	B	373	GLU	2.1
1	B	336	ALA	2.0
1	A	546	LEU	2.0
1	A	348	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

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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, 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.

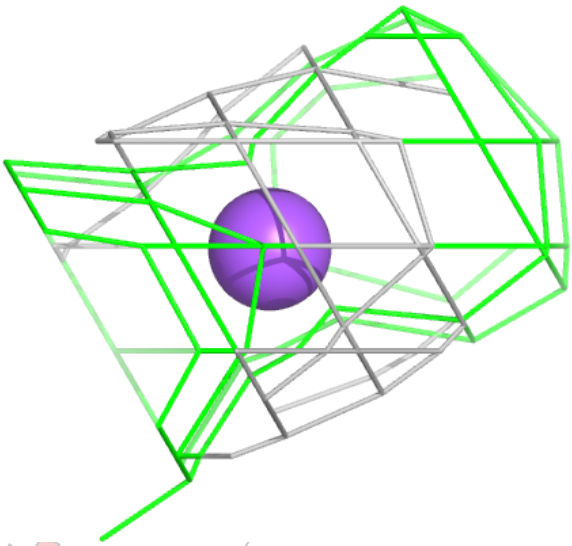
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	601	1/1	0.82	0.53	40,40,40,40	0
2	NA	B	602	1/1	0.95	0.55	65,65,65,65	0
2	NA	B	601	1/1	0.99	0.18	18,18,18,18	0

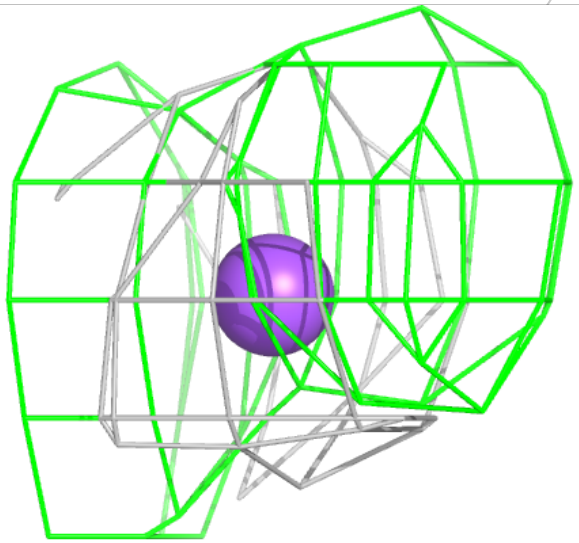
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

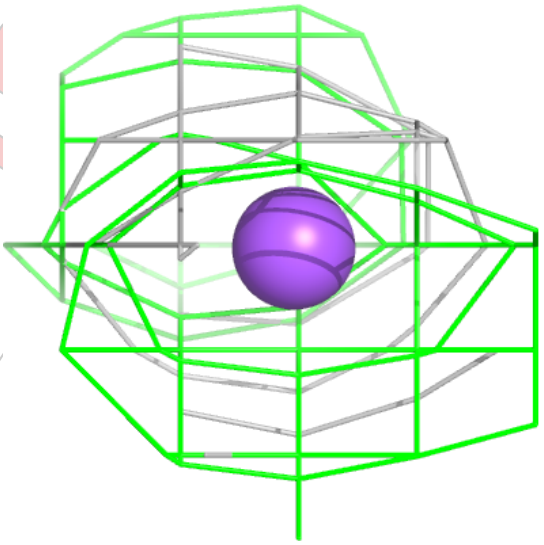
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Electron density around NA A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



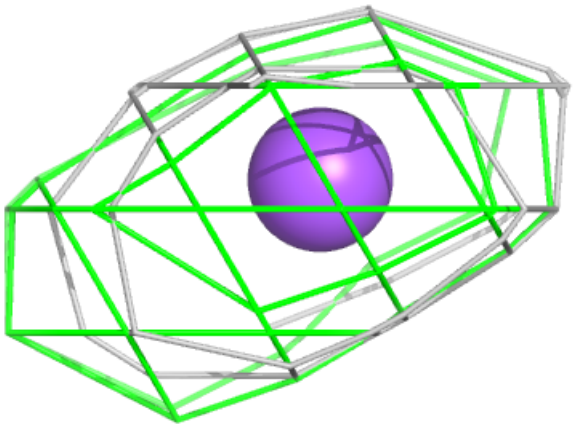


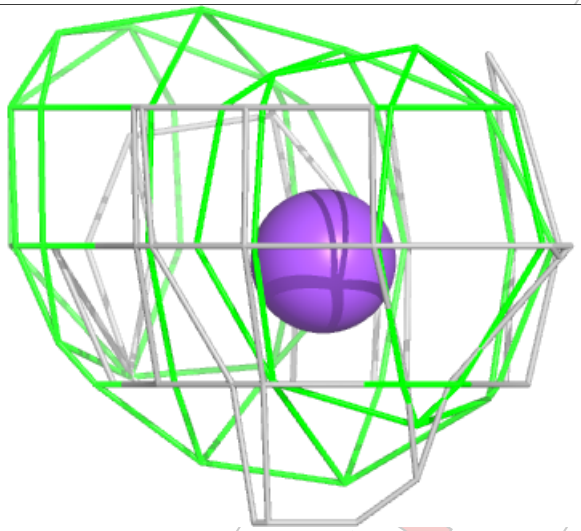


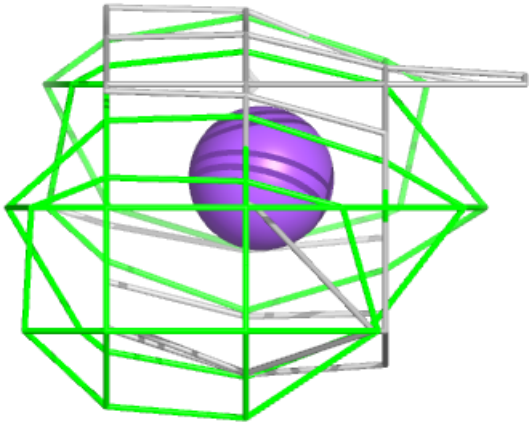
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Electron density around NA B 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



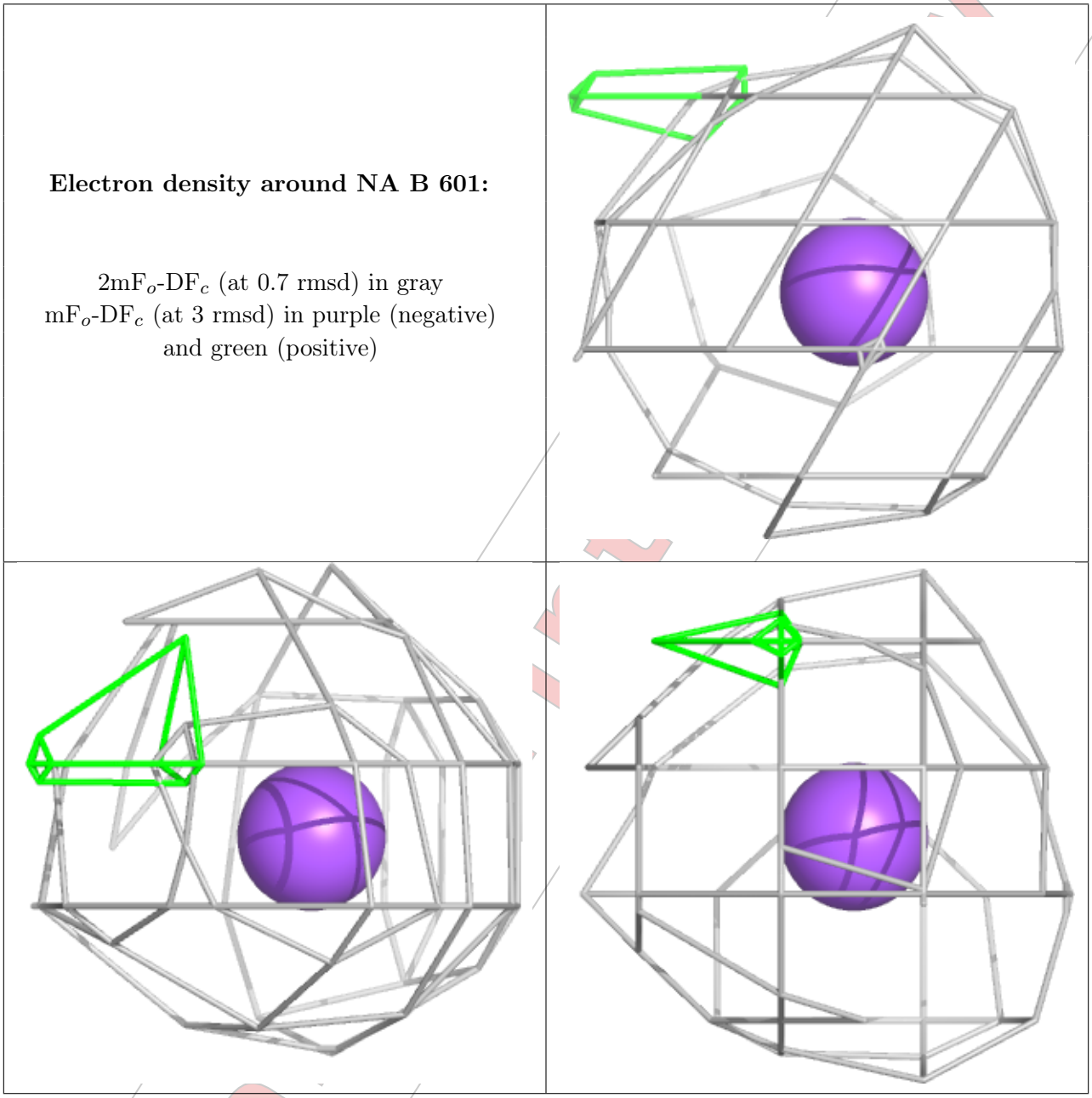




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Electron density around NA B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

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