wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:39 PM GMT

PDB ID	:	3RKI
Title	:	Structural basis for immunization with post-fusion RSV F to elicit high neutralizing antibody titers
Authors	:	Swanson, K.A.; Settembre, E.C.; Shaw, C.A.; Dey, A.K.; Rappuoli, R.; Mandl, C.W.; Dormitzer, P.D.; Carfi, A.
Deposited on	:	2011-04-18
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

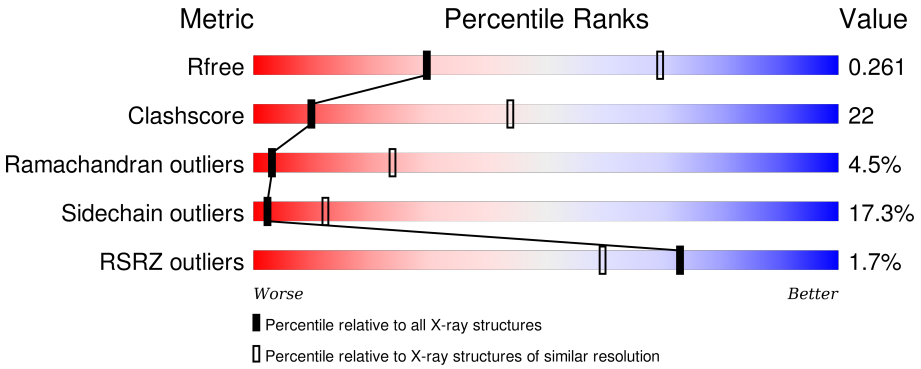
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	528	43% 30% 9% • 16%
1	B	528	43% 30% 8% • 17%
1	C	528	47% 27% 8% • 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1535	X	-	-	-
2	NAG	B	1535	X	-	-	-
2	NAG	C	1535	X	-	-	-
3	NAG	A	1525	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10438 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3424	2155	569	679	21			
1	B	439	Total	C	N	O	S	0	0	0
			3413	2149	567	676	21			
1	C	439	Total	C	N	O	S	0	0	0
			3419	2152	568	678	21			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	PRO	VARIANT	UNP P03420
A	?	-	PHE	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	?	-	PHE	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	LEU	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	?	-	VAL	DELETION	UNP P03420
A	?	-	GLY	DELETION	UNP P03420
A	379	VAL	ILE	VARIANT	UNP P03420
A	447	VAL	MET	VARIANT	UNP P03420
A	525	GLY	-	EXPRESSION TAG	UNP P03420
A	526	GLY	-	EXPRESSION TAG	UNP P03420
A	527	SER	-	EXPRESSION TAG	UNP P03420
A	528	ALA	-	EXPRESSION TAG	UNP P03420
A	529	GLY	-	EXPRESSION TAG	UNP P03420
A	530	SER	-	EXPRESSION TAG	UNP P03420
A	531	GLY	-	EXPRESSION TAG	UNP P03420
A	532	HIS	-	EXPRESSION TAG	UNP P03420
A	533	HIS	-	EXPRESSION TAG	UNP P03420
A	534	HIS	-	EXPRESSION TAG	UNP P03420
A	535	HIS	-	EXPRESSION TAG	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	536	HIS	-	EXPRESSION TAG	UNP P03420
A	537	HIS	-	EXPRESSION TAG	UNP P03420
B	111	ALA	PRO	VARIANT	UNP P03420
B	?	-	PHE	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	?	-	PHE	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	LEU	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	?	-	VAL	DELETION	UNP P03420
B	?	-	GLY	DELETION	UNP P03420
B	379	VAL	ILE	VARIANT	UNP P03420
B	447	VAL	MET	VARIANT	UNP P03420
B	525	GLY	-	EXPRESSION TAG	UNP P03420
B	526	GLY	-	EXPRESSION TAG	UNP P03420
B	527	SER	-	EXPRESSION TAG	UNP P03420
B	528	ALA	-	EXPRESSION TAG	UNP P03420
B	529	GLY	-	EXPRESSION TAG	UNP P03420
B	530	SER	-	EXPRESSION TAG	UNP P03420
B	531	GLY	-	EXPRESSION TAG	UNP P03420
B	532	HIS	-	EXPRESSION TAG	UNP P03420
B	533	HIS	-	EXPRESSION TAG	UNP P03420
B	534	HIS	-	EXPRESSION TAG	UNP P03420
B	535	HIS	-	EXPRESSION TAG	UNP P03420
B	536	HIS	-	EXPRESSION TAG	UNP P03420
B	537	HIS	-	EXPRESSION TAG	UNP P03420
C	111	ALA	PRO	VARIANT	UNP P03420
C	?	-	PHE	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	?	-	PHE	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	LEU	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	?	-	VAL	DELETION	UNP P03420
C	?	-	GLY	DELETION	UNP P03420
C	379	VAL	ILE	VARIANT	UNP P03420
C	447	VAL	MET	VARIANT	UNP P03420
C	525	GLY	-	EXPRESSION TAG	UNP P03420
C	526	GLY	-	EXPRESSION TAG	UNP P03420
C	527	SER	-	EXPRESSION TAG	UNP P03420

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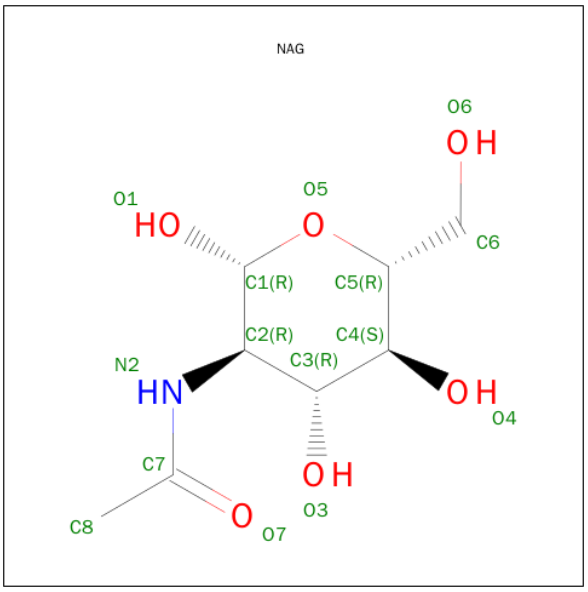
Chain	Residue	Modelled	Actual	Comment	Reference
C	528	ALA	-	EXPRESSION TAG	UNP P03420
C	529	GLY	-	EXPRESSION TAG	UNP P03420
C	530	SER	-	EXPRESSION TAG	UNP P03420
C	531	GLY	-	EXPRESSION TAG	UNP P03420
C	532	HIS	-	EXPRESSION TAG	UNP P03420
C	533	HIS	-	EXPRESSION TAG	UNP P03420
C	534	HIS	-	EXPRESSION TAG	UNP P03420
C	535	HIS	-	EXPRESSION TAG	UNP P03420
C	536	HIS	-	EXPRESSION TAG	UNP P03420
C	537	HIS	-	EXPRESSION TAG	UNP P03420

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

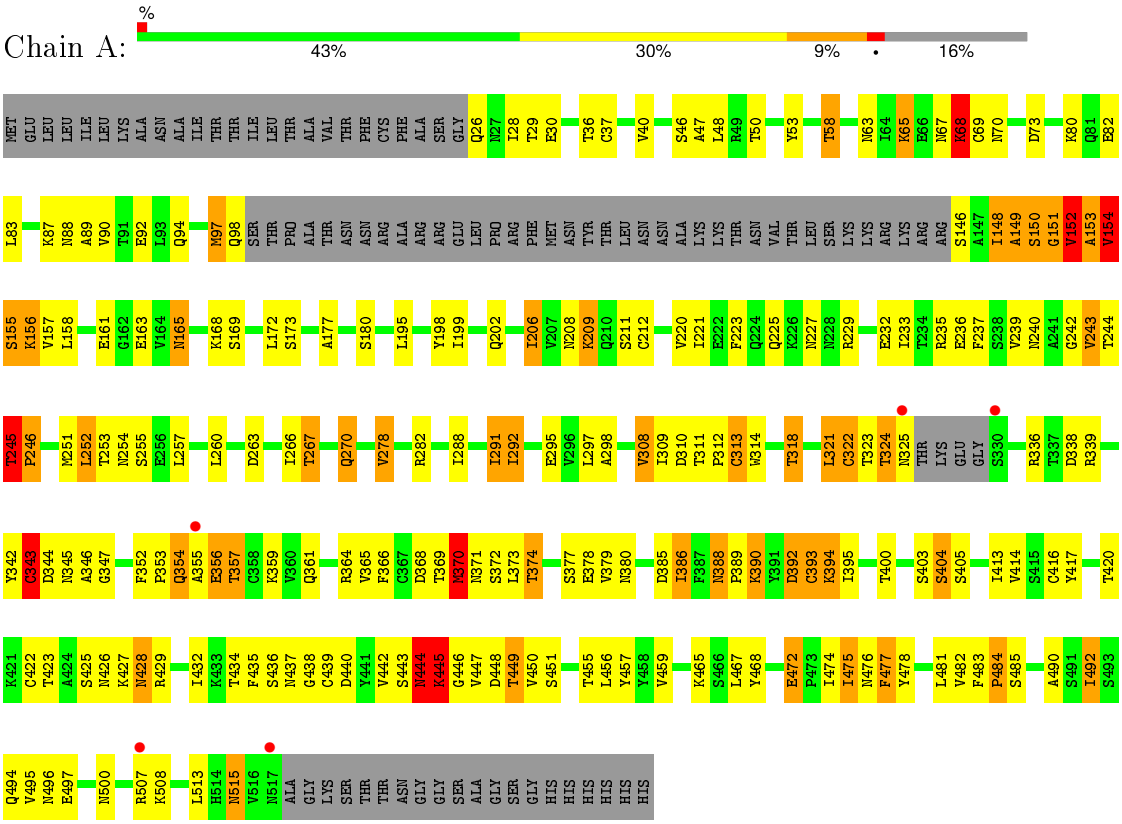


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0

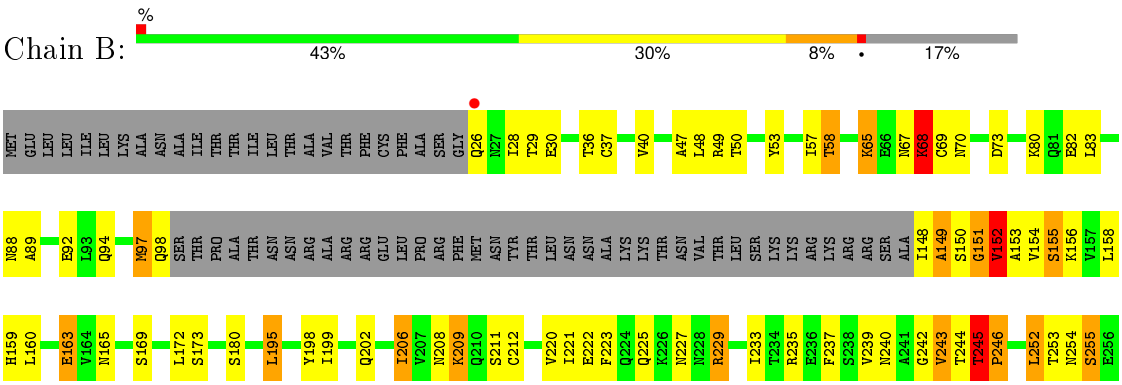
3 Residue-property plots (i)

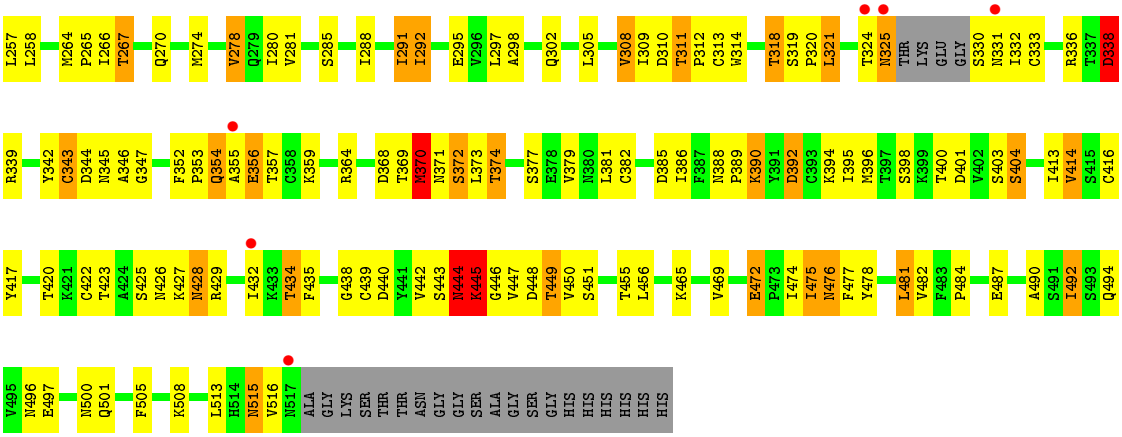
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Fusion glycoprotein F0



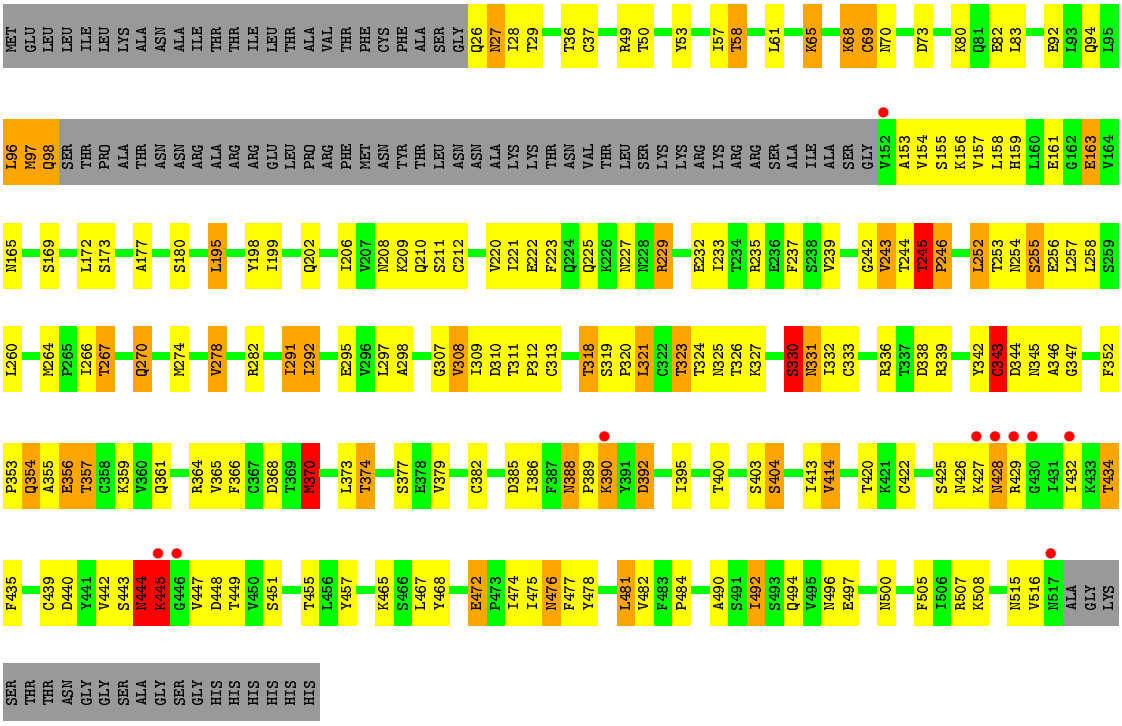
- Molecule 1: Fusion glycoprotein F0





• Molecule 1: Fusion glycoprotein F0

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.93Å 113.16Å 311.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.0 (30.00-3.20) 77.1 (29.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.264 0.225 , 0.261	Depositor DCC
R_{free} test set	2065 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 40186 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10438	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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

5.1 Standard geometry

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

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	1.05	9/3471 (0.3%)	0.95	6/4703 (0.1%)
1	B	0.84	2/3460 (0.1%)	0.86	3/4688 (0.1%)
1	C	0.93	3/3467 (0.1%)	0.92	5/4698 (0.1%)
All	All	0.94	14/10398 (0.1%)	0.91	14/14089 (0.1%)

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	6
1	B	0	5
1	C	0	5
2	A	1	0
2	B	1	0
2	C	1	0
All	All	3	16

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	CYS	CB-SG	-11.88	1.62	1.82
1	A	313	CYS	CB-SG	-8.06	1.68	1.82
1	C	343	CYS	CB-SG	-7.20	1.70	1.82
1	A	393	CYS	CB-SG	-6.42	1.71	1.82
1	A	322	CYS	CB-SG	-6.38	1.71	1.82

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	245	THR	C-N-CD	-9.15	100.46	120.60
1	B	245	THR	C-N-CD	-7.10	104.98	120.60
1	A	245	THR	C-N-CD	-7.01	105.19	120.60
1	A	212	CYS	CA-CB-SG	-6.72	101.90	114.00
1	B	212	CYS	CA-CB-SG	-5.90	103.38	114.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1535	NAG	C1
2	B	1535	NAG	C1
2	C	1535	NAG	C1

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	VAL	Peptide
1	A	245	THR	Peptide
1	A	392	ASP	Peptide
1	A	444	ASN	Peptide
1	A	445	LYS	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	3424	0	3456	193	1
1	B	3413	0	3447	178	0
1	C	3419	0	3453	173	0
2	A	56	0	50	0	0
2	B	56	0	50	2	0
2	C	56	0	50	1	0
3	A	14	0	13	0	0
All	All	10438	0	10519	462	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 22.

The worst 5 of 462 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:154:VAL:CG1	1:A:155:SER:H	1.46	1.26
1:A:154:VAL:HG13	1:A:155:SER:H	1.07	1.09
1:A:65:LYS:HZ2	1:B:475:ILE:HA	0.97	1.08
1:A:475:ILE:O	1:A:477:PHE:HD2	1.35	1.07
1:B:475:ILE:O	1:B:477:PHE:HD2	1.37	1.07

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:A:150:SER:CB	1:A:395:ILE:O[2_555]	2.09	0.11

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	435/528 (82%)	370 (85%)	43 (10%)	22 (5%)	2	20
1	B	433/528 (82%)	366 (84%)	49 (11%)	18 (4%)	3	26
1	C	435/528 (82%)	371 (85%)	45 (10%)	19 (4%)	3	24
All	All	1303/1584 (82%)	1107 (85%)	137 (10%)	59 (4%)	3	24

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	149	ALA
1	A	150	SER
1	A	153	ALA
1	A	246	PRO

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	406/477 (85%)	339 (84%)	67 (16%)	3 13
1	B	405/477 (85%)	329 (81%)	76 (19%)	2 10
1	C	406/477 (85%)	338 (83%)	68 (17%)	3 13
All	All	1217/1431 (85%)	1006 (83%)	211 (17%)	2 12

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	288	ILE
1	B	403	SER
1	C	432	ILE
1	B	295	GLU
1	B	354	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	ASN
1	B	325	ASN
1	C	345	ASN
1	B	270	GLN
1	B	388	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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 (i)

12 carbohydrates 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	NAG	A	1535	1,2	14,14,15	0.95	0	15,19,21	2.46	6 (40%)
2	NAG	A	1536	2	14,14,15	0.94	1 (7%)	15,19,21	2.02	4 (26%)
2	NAG	A	1545	1,2	14,14,15	1.24	1 (7%)	15,19,21	2.07	5 (33%)
2	NAG	A	1546	2	14,14,15	1.01	1 (7%)	15,19,21	3.20	3 (20%)
2	NAG	B	1535	1,2	14,14,15	1.02	1 (7%)	15,19,21	1.88	3 (20%)
2	NAG	B	1536	2	14,14,15	1.39	1 (7%)	15,19,21	1.55	3 (20%)
2	NAG	B	1545	1,2	14,14,15	0.83	1 (7%)	15,19,21	1.74	5 (33%)
2	NAG	B	1546	2	14,14,15	1.57	3 (21%)	15,19,21	2.99	6 (40%)
2	NAG	C	1535	1,2	14,14,15	1.44	1 (7%)	15,19,21	2.76	4 (26%)
2	NAG	C	1536	2	14,14,15	1.04	1 (7%)	15,19,21	1.78	2 (13%)
2	NAG	C	1545	1,2	14,14,15	1.31	1 (7%)	15,19,21	3.24	7 (46%)
2	NAG	C	1546	2	14,14,15	0.96	1 (7%)	15,19,21	2.07	2 (13%)

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	NAG	A	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1536	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1546	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1536	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1546	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1535	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1536	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1545	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1546	2	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1536	NAG	C1-C2	2.10	1.55	1.52
2	B	1546	NAG	C3-C2	2.22	1.57	1.52
2	B	1545	NAG	C1-C2	2.37	1.55	1.52
2	A	1545	NAG	C4-C5	2.57	1.58	1.53
2	B	1535	NAG	C1-C2	2.59	1.56	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1545	NAG	C4-C3-C2	-3.89	105.17	111.23
2	A	1535	NAG	O7-C7-C8	-2.93	116.68	122.06
2	B	1546	NAG	O7-C7-C8	-2.89	116.75	122.06
2	C	1545	NAG	C3-C4-C5	-2.85	105.22	110.20
2	C	1535	NAG	O7-C7-C8	-2.17	118.08	122.06

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1535	NAG	C1
2	C	1535	NAG	C1
2	B	1535	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1535	NAG	2	0
2	B	1536	NAG	1	0
2	C	1535	NAG	1	0

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	$\#\|Z\| > 2$
3	NAG	A	1525	1	14,14,15	2.30	3 (21%)	15,19,21	3.58	7 (46%)

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
3	NAG	A	1525	1	1/1/5/7	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1525	NAG	C3-C2	3.10	1.59	1.52
3	A	1525	NAG	C2-N2	3.72	1.52	1.46
3	A	1525	NAG	C1-C2	6.27	1.61	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1525	NAG	O7-C7-C8	-2.90	116.74	122.06
3	A	1525	NAG	O7-C7-N2	2.27	126.48	121.86
3	A	1525	NAG	O5-C5-C6	2.72	113.24	107.35
3	A	1525	NAG	O3-C3-C2	2.91	114.87	109.11
3	A	1525	NAG	C6-C5-C4	3.40	121.40	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1525	NAG	C1

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.

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	441/528 (83%)	-0.47	5 (1%)	82	72	22, 47, 89, 116	5 (1%)
1	B	439/528 (83%)	-0.33	7 (1%)	74	62	28, 62, 91, 108	5 (1%)
1	C	439/528 (83%)	-0.27	10 (2%)	64	49	18, 57, 114, 137	5 (1%)
All	All	1319/1584 (83%)	-0.36	22 (1%)	73	60	18, 55, 101, 137	15 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	ASN	4.8
1	B	324	THR	4.5
1	B	325	ASN	4.4
1	B	432	ILE	3.7
1	C	432	ILE	3.5

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

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	NAG	C	1536	14/15	0.70	0.62	-	101,103,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	1536	14/15	0.77	0.56	-	106,109,110,110	0
2	NAG	A	1535	14/15	0.89	0.50	-	80,91,95,101	0
2	NAG	C	1546	14/15	0.78	0.45	-	88,93,96,97	0
2	NAG	A	1545	14/15	0.77	0.39	-	63,75,79,85	0
2	NAG	C	1535	14/15	0.83	0.45	-	76,87,91,96	0
2	NAG	B	1546	14/15	0.58	0.49	-	93,95,98,99	0
2	NAG	C	1545	14/15	0.83	0.32	-	67,80,84,87	0
2	NAG	B	1536	14/15	0.72	0.54	-	104,106,109,110	0
2	NAG	B	1545	14/15	0.87	0.28	-	66,78,83,86	0
2	NAG	A	1546	14/15	0.83	0.51	-	90,93,95,96	0
2	NAG	B	1535	14/15	0.77	0.46	-	78,87,92,99	0

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, 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
3	NAG	A	1525	14/15	0.74	0.43	-	51,61,64,66	0

6.5 Other polymers

There are no such residues in this entry.