



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:01 AM GMT

PDB ID : 3GVK
Title : Crystal structure of endo-neuraminidase NF mutant
Authors : Schulz, E.C.; Dickmanns, A.; Ficner, R.
Deposited on : 2009-03-31
Resolution : 1.84 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

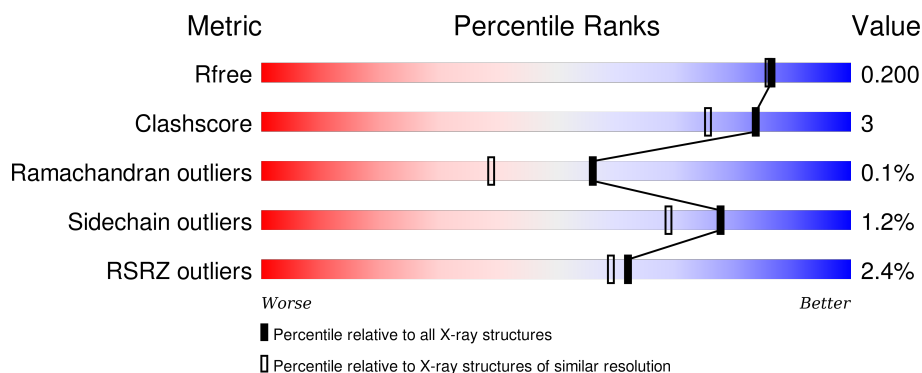
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

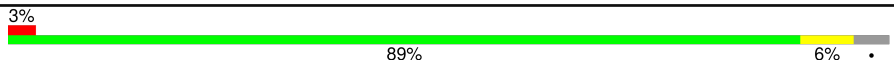
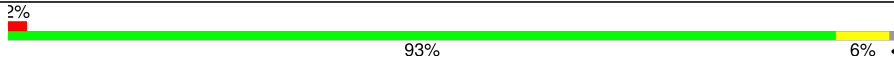
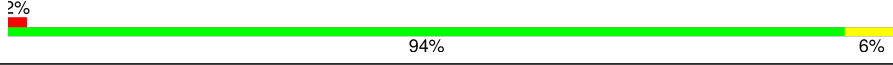
The reported resolution of this entry is 1.84 Å.

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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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 $\leq 5\%$. 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	670	
1	B	670	
1	C	670	

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	SLB	A	1	-	-	-	X
2	SLB	B	1	-	-	-	X
2	SLB	B	911	-	-	-	X
2	SLB	C	1	-	-	-	X
2	SIA	C	2	-	-	-	X
3	SLB	A	914	-	-	-	X
3	SLB	B	914	-	-	-	X
3	SIA	B	915	-	-	-	X
3	SLB	C	914	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18367 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 Endo-N-acetylneuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	17	0
			5163	3266	892	985	20			
1	B	666	Total	C	N	O	S	0	14	0
			5295	3341	911	1023	20			
1	C	666	Total	C	N	O	S	0	12	0
			5287	3335	916	1016	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	VAL	-	expression tag	UNP Q858B1
A	242	PRO	-	expression tag	UNP Q858B1
A	243	ARG	-	expression tag	UNP Q858B1
A	244	GLY	-	expression tag	UNP Q858B1
A	245	SER	-	expression tag	UNP Q858B1
A	350	ALA	HIS	engineered	UNP Q858B1
B	241	VAL	-	expression tag	UNP Q858B1
B	242	PRO	-	expression tag	UNP Q858B1
B	243	ARG	-	expression tag	UNP Q858B1
B	244	GLY	-	expression tag	UNP Q858B1
B	245	SER	-	expression tag	UNP Q858B1
B	350	ALA	HIS	engineered	UNP Q858B1
C	241	VAL	-	expression tag	UNP Q858B1
C	242	PRO	-	expression tag	UNP Q858B1
C	243	ARG	-	expression tag	UNP Q858B1
C	244	GLY	-	expression tag	UNP Q858B1
C	245	SER	-	expression tag	UNP Q858B1
C	350	ALA	HIS	engineered	UNP Q858B1

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			61	33	3	25		
2	A	3	Total	C	N	O	0	0
			61	33	3	25		
2	B	3	Total	C	N	O	0	0
			61	33	3	25		
2	B	3	Total	C	N	O	0	0
			61	33	3	25		
2	C	3	Total	C	N	O	0	0
			61	33	3	25		
2	C	3	Total	C	N	O	0	0
			61	33	3	25		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			41	22	2	17		
3	B	2	Total	C	N	O	0	0
			41	22	2	17		
3	C	2	Total	C	N	O	0	0
			41	22	2	17		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

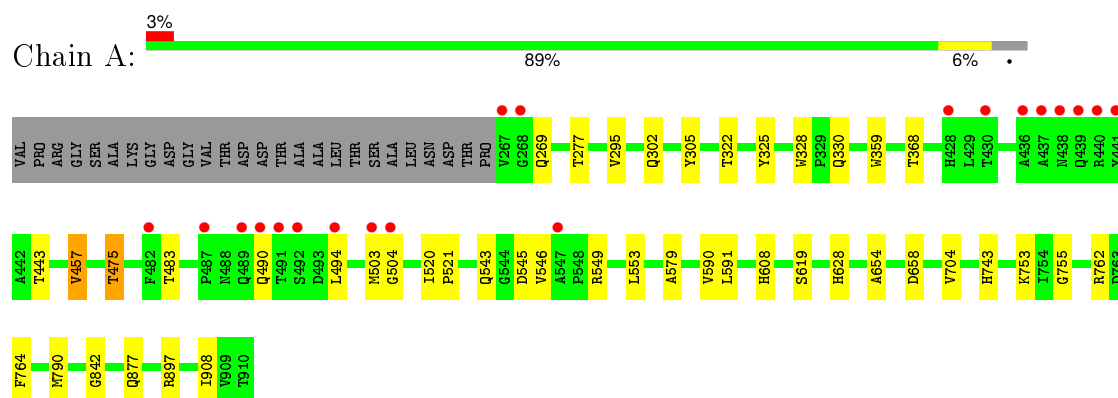
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	625	Total	O	0	0
			625	625		
5	B	767	Total	O	0	0
			767	767		
5	C	738	Total	O	0	0
			738	738		

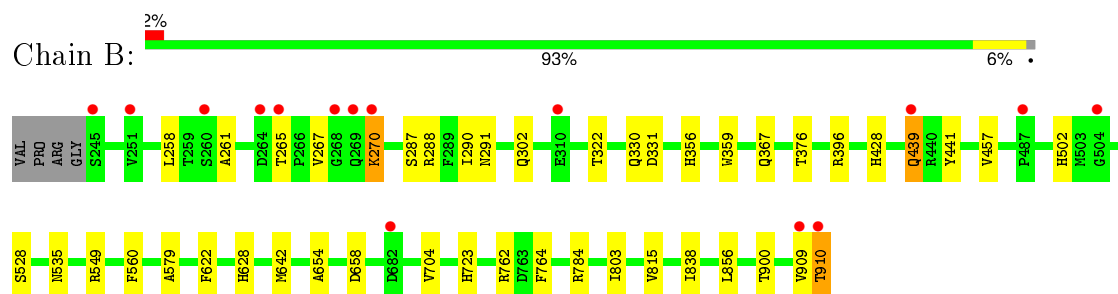
3 Residue-property plots [i](#)

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.

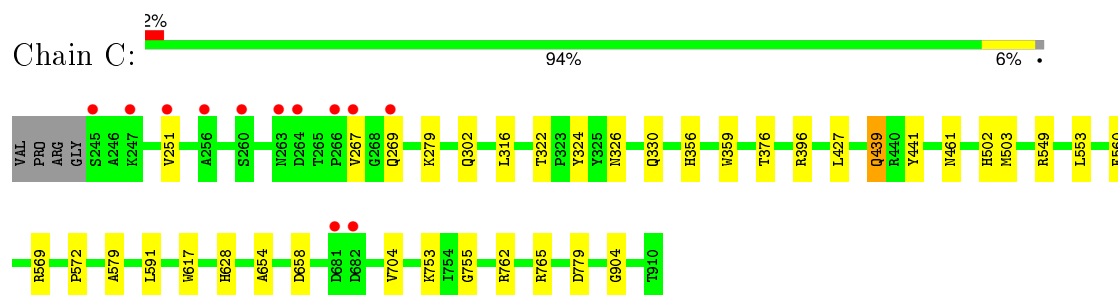
• Molecule 1: Endo-N-acetylneuraminidase



• Molecule 1: Endo-N-acetylneuraminidase



• Molecule 1: Endo-N-acetylneuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.40 Å 153.70 Å 157.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.84 19.81 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.84) 99.9 (19.81-1.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.08 (at 1.84 Å)	Xtriage
Refinement program	REFMAC 5.5.0039	Depositor
R, R_{free}	0.265 , 0.282 0.170 , 0.200	Depositor DCC
R_{free} test set	9487 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 189954 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18367	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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, 0.375 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: NA, SIA, SLB

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	0.37	0/5360	0.53	0/7301
1	B	0.38	0/5479	0.54	0/7463
1	C	0.37	0/5469	0.53	0/7450
All	All	0.37	0/16308	0.54	0/22214

There are no bond length outliers.

There are no bond angle outliers.

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	5163	0	4929	31	0
1	B	5295	0	5039	38	0
1	C	5287	0	5040	27	0
2	A	122	0	98	3	0
2	B	122	0	100	2	0
2	C	122	0	99	4	0
3	A	41	0	34	2	0
3	B	41	0	34	1	0
3	C	41	0	34	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	625	0	0	3	0
5	B	767	0	0	5	0
5	C	738	0	0	3	0
All	All	18367	0	15407	94	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 3.

All (94) 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:543:GLN:HE22	1:A:546:VAL:H	1.23	0.86
1:B:302:GLN:HE22	1:B:654:ALA:H	1.26	0.83
1:C:302:GLN:HE22	1:C:654:ALA:H	1.29	0.80
3:A:914:SLB:H92	3:A:914:SLB:O6	1.84	0.78
1:B:367:GLN:HE22	1:B:764:PHE:H	1.33	0.76
1:A:302:GLN:HE22	1:A:654:ALA:H	1.33	0.73
1:A:897:ARG:HH11	1:B:910[A]:THR:HG22	1.54	0.72
1:B:367:GLN:HE21	1:C:765:ARG:HH22	1.36	0.72
1:C:322:THR:HG22	1:C:324:TYR:H	1.55	0.72
1:A:628:HIS:HE1	1:A:658:ASP:OD1	1.76	0.68
1:A:475:THR:HG22	1:A:483:THR:OG1	2.02	0.58
1:B:628:HIS:HE1	1:B:658:ASP:OD1	1.87	0.58
1:B:910[A]:THR:HG23	1:C:904:GLY:HA2	1.86	0.57
1:C:396:ARG:HB3	1:C:560:PHE:CZ	2.40	0.56
1:A:330:GLN:HB3	1:A:704:VAL:O	2.04	0.56
2:A:1:SLB:H112	2:A:1:SLB:H6	1.88	0.55
1:B:302:GLN:HE22	1:B:654:ALA:N	2.01	0.54
1:C:322:THR:HB	1:C:326:ASN:OD1	2.07	0.54
1:B:723:HIS:HE1	5:B:1936:HOH:O	1.89	0.54
1:C:322:THR:HG21	5:C:1028:HOH:O	2.09	0.53
1:B:396:ARG:HB3	1:B:560:PHE:CZ	2.44	0.53
1:B:428:HIS:ND1	1:B:502:HIS:HD2	2.06	0.53
1:C:549:ARG:HD3	1:C:579:ALA:O	2.08	0.53
1:A:628:HIS:HD2	5:A:987:HOH:O	1.92	0.52
1:A:842:GLY:HA2	1:B:838[B]:ILE:CD1	2.39	0.52
1:B:910[A]:THR:CG2	1:C:904:GLY:HA2	2.39	0.52
1:B:356:HIS:HE1	5:B:13:HOH:O	1.92	0.52
1:A:543:GLN:NE2	1:A:545:ASP:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HA	1:A:504:GLY:O	2.09	0.51
1:C:569[A]:ARG:HG3	1:C:569[A]:ARG:HH21	1.74	0.51
1:B:367:GLN:HE21	1:C:765:ARG:NH2	2.06	0.51
1:A:443[A]:THR:HG22	1:A:483:THR:HG22	1.93	0.51
1:B:838[B]:ILE:HD11	1:B:856:LEU:HB2	1.91	0.51
1:A:764:PHE:HB3	1:C:316:LEU:HD23	1.93	0.50
1:C:302:GLN:HE22	1:C:654:ALA:N	2.03	0.50
1:B:549:ARG:HD3	1:B:579:ALA:O	2.12	0.50
1:B:622:PHE:CZ	1:B:642[B]:MET:HE1	2.48	0.49
1:A:790[B]:MET:HG2	1:B:784:ARG:HB2	1.95	0.49
1:C:628:HIS:HE1	1:C:658:ASP:OD1	1.95	0.49
1:A:842:GLY:HA2	1:B:838[B]:ILE:HD12	1.95	0.49
1:B:330:GLN:HB3	1:B:704:VAL:O	2.13	0.49
1:C:356:HIS:HE1	5:C:6:HOH:O	1.96	0.49
1:B:261:ALA:O	1:B:265:THR:HG22	2.14	0.48
1:A:269:GLN:HE22	1:B:291:ASN:HD21	1.62	0.48
1:B:838[B]:ILE:CD1	1:B:856:LEU:HB2	2.44	0.48
1:B:356:HIS:HD2	1:B:376:THR:O	1.97	0.48
1:A:908:ILE:HD12	1:B:900:THR:HG21	1.95	0.48
2:B:1:SLB:C1	5:B:1949:HOH:O	2.61	0.48
1:A:295[A]:VAL:HG22	1:A:305:TYR:CE1	2.48	0.47
1:C:753:LYS:HE2	1:C:755:GLY:O	2.14	0.47
1:A:549:ARG:HD3	1:A:579:ALA:O	2.14	0.47
2:C:911:SLB:O6	2:C:911:SLB:H92	2.15	0.47
1:C:427:LEU:N	1:C:503:MET:O	2.27	0.46
1:B:838[B]:ILE:HD13	1:B:838[B]:ILE:H	1.80	0.46
1:C:356:HIS:HD2	1:C:376:THR:O	1.98	0.46
1:A:608:HIS:HD2	1:A:619:SER:OG	1.98	0.46
1:A:328:TRP:HD1	1:A:330:GLN:HE21	1.64	0.46
1:A:368[A]:THR:CG2	5:A:1197:HOH:O	2.63	0.46
1:A:753:LYS:HE2	1:A:755:GLY:O	2.16	0.46
1:A:302:GLN:HE22	1:A:654:ALA:N	2.06	0.46
1:A:743:HIS:HD2	5:A:940:HOH:O	1.99	0.45
1:B:367:GLN:NE2	1:C:765:ARG:HH22	2.08	0.45
1:A:877:GLN:NE2	3:B:914:SLB:O7	2.50	0.45
1:B:909:VAL:HA	1:B:910[B]:THR:HA	1.80	0.45
1:C:330:GLN:HB3	1:C:704:VAL:O	2.16	0.44
2:C:1:SLB:O10	2:C:2:SIA:H91	2.18	0.44
1:B:628:HIS:HD2	5:B:941:HOH:O	2.00	0.44
1:B:909:VAL:HG12	1:B:910[B]:THR:HG22	2.00	0.44
1:C:439:GLN:HE22	1:C:441:TYR:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1:SLB:O6	2:C:1:SLB:H91	2.18	0.43
1:B:439[A]:GLN:NE2	1:B:441:TYR:H	2.15	0.43
1:B:439[A]:GLN:HE22	1:B:441:TYR:HB2	1.83	0.43
1:B:287:SER:OG	1:C:753:LYS:HE3	2.19	0.43
2:C:1:SLB:O7	2:C:1:SLB:N5	2.51	0.43
1:A:490:GLN:HB2	1:A:494:LEU:HD11	2.01	0.42
2:A:1:SLB:C11	2:A:1:SLB:H6	2.50	0.42
1:A:553:LEU:HD22	1:A:591[A]:LEU:HD21	2.00	0.42
5:B:1179:HOH:O	1:C:779:ASP:HB2	2.19	0.42
1:C:553:LEU:HD22	1:C:591[A]:LEU:HD21	2.01	0.42
3:A:914:SLB:C9	3:A:914:SLB:O6	2.58	0.42
2:B:1:SLB:O6	2:B:1:SLB:H92	2.20	0.42
1:C:572:PRO:HD3	1:C:617:TRP:CD1	2.55	0.42
1:B:265:THR:HG23	1:B:288:ARG:HH11	1.84	0.41
1:C:461:ASN:HD22	1:C:502:HIS:HD2	1.68	0.41
1:C:251:VAL:O	1:C:279:LYS:HD2	2.20	0.41
1:A:368[A]:THR:HG21	5:C:1140:HOH:O	2.20	0.41
1:B:331:ASP:HB3	1:B:528:SER:HA	2.01	0.41
1:A:503:MET:HG2	1:A:504:GLY:HA3	2.03	0.41
2:A:1:SLB:H112	2:A:1:SLB:C6	2.51	0.41
1:B:270:LYS:HB3	1:B:290:ILE:HG12	2.02	0.41
1:A:277:THR:HG22	1:A:295[A]:VAL:HG23	2.02	0.41
1:B:803[B]:ILE:HD13	1:B:815:VAL:CG2	2.50	0.41
1:A:520:ILE:HA	1:A:521:PRO:HD3	1.96	0.40
1:B:396:ARG:HH21	1:B:535:ASN:HD22	1.68	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	659/670 (98%)	633 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	677/670 (101%)	654 (97%)	23 (3%)	0	100	100
1	C	676/670 (101%)	650 (96%)	25 (4%)	1 (0%)	56	39
All	All	2012/2010 (100%)	1937 (96%)	74 (4%)	1 (0%)	56	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	267	VAL

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	564/566 (100%)	557 (99%)	7 (1%)	78	69
1	B	577/566 (102%)	566 (98%)	11 (2%)	65	50
1	C	575/566 (102%)	571 (99%)	4 (1%)	88	84
All	All	1716/1698 (101%)	1694 (99%)	22 (1%)	78	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	THR
1	A	325	TYR
1	A	359	TRP
1	A	457	VAL
1	A	475	THR
1	A	590	VAL
1	A	762	ARG
1	B	258	LEU
1	B	267	VAL
1	B	270	LYS
1	B	322	THR
1	B	359	TRP
1	B	439[A]	GLN

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Mol	Chain	Res	Type
1	B	439[B]	GLN
1	B	457	VAL
1	B	762	ARG
1	B	910[A]	THR
1	B	910[B]	THR
1	C	269	GLN
1	C	359	TRP
1	C	439	GLN
1	C	762	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	274	ASN
1	A	302	GLN
1	A	326	ASN
1	A	330	GLN
1	A	388	HIS
1	A	397	ASN
1	A	461	ASN
1	A	490	GLN
1	A	502	HIS
1	A	535	ASN
1	A	543	GLN
1	A	608	HIS
1	A	628	HIS
1	A	676	ASN
1	A	699	ASN
1	A	743	HIS
1	A	853	GLN
1	B	269	GLN
1	B	302	GLN
1	B	326	ASN
1	B	338	ASN
1	B	356	HIS
1	B	367	GLN
1	B	397	ASN
1	B	415	ASN
1	B	445	HIS
1	B	461	ASN
1	B	502	HIS

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Mol	Chain	Res	Type
1	B	535	ASN
1	B	570	GLN
1	B	628	HIS
1	B	676	ASN
1	B	723	HIS
1	B	853	GLN
1	C	269	GLN
1	C	302	GLN
1	C	338	ASN
1	C	356	HIS
1	C	415	ASN
1	C	438	ASN
1	C	439	GLN
1	C	461	ASN
1	C	608	HIS
1	C	628	HIS
1	C	699	ASN
1	C	853	GLN
1	C	896	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 ⓘ

24 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	SLB	A	1	2	17,21,21	1.17	2 (11%)	19,31,31	5.16	5 (26%)
2	SIA	A	2	1,2	16,20,21	0.48	0	18,28,31	1.21	2 (11%)
2	SIA	A	3	2	16,20,21	0.42	0	18,28,31	1.07	2 (11%)
2	SLB	A	911	2	17,21,21	1.08	1 (5%)	19,31,31	5.54	3 (15%)
2	SIA	A	912	2	16,20,21	0.33	0	18,28,31	1.19	2 (11%)
2	SIA	A	913	2	16,20,21	0.36	0	18,28,31	1.11	2 (11%)
3	SLB	A	914	3	17,21,21	0.95	1 (5%)	19,31,31	5.53	3 (15%)
3	SIA	A	915	3	16,20,21	0.44	0	18,28,31	0.98	1 (5%)
2	SLB	B	1	2	17,21,21	1.80	3 (17%)	19,31,31	4.95	3 (15%)
2	SIA	B	2	2	16,20,21	0.37	0	18,28,31	1.02	1 (5%)
2	SIA	B	3	2	16,20,21	0.27	0	18,28,31	0.94	2 (11%)
2	SLB	B	911	2	17,21,21	1.06	1 (5%)	19,31,31	5.40	4 (21%)
2	SIA	B	912	2	16,20,21	0.34	0	18,28,31	1.18	2 (11%)
2	SIA	B	913	2	16,20,21	0.39	0	18,28,31	0.95	2 (11%)
3	SLB	B	914	3	17,21,21	1.14	1 (5%)	19,31,31	5.64	4 (21%)
3	SIA	B	915	3	16,20,21	0.39	0	18,28,31	1.11	1 (5%)
2	SLB	C	1	2	17,21,21	1.63	3 (17%)	19,31,31	6.43	9 (47%)
2	SIA	C	2	2	16,20,21	0.43	0	18,28,31	1.03	2 (11%)
2	SIA	C	3	2	16,20,21	0.32	0	18,28,31	1.07	2 (11%)
2	SLB	C	911	2	17,21,21	1.24	1 (5%)	19,31,31	5.24	2 (10%)
2	SIA	C	912	2	16,20,21	0.37	0	18,28,31	1.09	1 (5%)
2	SIA	C	913	2	16,20,21	0.39	0	18,28,31	1.05	2 (11%)
3	SLB	C	914	3	17,21,21	1.25	1 (5%)	19,31,31	5.41	2 (10%)
3	SIA	C	915	3	16,20,21	0.37	0	18,28,31	1.02	2 (11%)

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	SLB	A	1	2	-	0/14/38/38	0/1/1/1
2	SIA	A	2	1,2	-	0/14/34/38	0/1/1/1
2	SIA	A	3	2	-	0/14/34/38	0/1/1/1
2	SLB	A	911	2	-	0/14/38/38	0/1/1/1
2	SIA	A	912	2	-	0/14/34/38	0/1/1/1
2	SIA	A	913	2	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SLB	A	914	3	-	0/14/38/38	0/1/1/1
3	SIA	A	915	3	-	0/14/34/38	0/1/1/1
2	SLB	B	1	2	-	0/14/38/38	0/1/1/1
2	SIA	B	2	2	-	0/14/34/38	0/1/1/1
2	SIA	B	3	2	-	0/14/34/38	0/1/1/1
2	SLB	B	911	2	-	0/14/38/38	0/1/1/1
2	SIA	B	912	2	-	0/14/34/38	0/1/1/1
2	SIA	B	913	2	-	0/14/34/38	0/1/1/1
3	SLB	B	914	3	-	0/14/38/38	0/1/1/1
3	SIA	B	915	3	-	0/14/34/38	0/1/1/1
2	SLB	C	1	2	-	0/14/38/38	0/1/1/1
2	SIA	C	2	2	-	0/14/34/38	0/1/1/1
2	SIA	C	3	2	-	0/14/34/38	0/1/1/1
2	SLB	C	911	2	-	0/14/38/38	0/1/1/1
2	SIA	C	912	2	-	0/14/34/38	0/1/1/1
2	SIA	C	913	2	-	0/14/34/38	0/1/1/1
3	SLB	C	914	3	-	0/14/38/38	0/1/1/1
3	SIA	C	915	3	-	0/14/34/38	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SLB	O6-C2	-5.19	1.38	1.42
2	C	1	SLB	O6-C6	-3.19	1.38	1.44
2	B	1	SLB	O6-C6	-2.28	1.40	1.44
2	A	1	SLB	O6-C2	-2.14	1.40	1.42
2	C	1	SLB	C3-C2	2.09	1.54	1.51
3	A	914	SLB	O2-C2	3.44	1.43	1.40
2	A	1	SLB	O2-C2	3.48	1.43	1.40
2	A	911	SLB	O2-C2	3.69	1.43	1.40
3	B	914	SLB	O2-C2	3.81	1.44	1.40
2	B	1	SLB	O2-C2	4.03	1.44	1.40
2	B	911	SLB	O2-C2	4.07	1.44	1.40
3	C	914	SLB	O2-C2	4.27	1.44	1.40
2	C	1	SLB	O2-C2	4.33	1.44	1.40
2	C	911	SLB	O2-C2	4.48	1.44	1.40

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	SLB	O2-C2-C3	-23.52	80.04	109.41
3	B	914	SLB	O2-C2-C3	-19.07	85.59	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	914	SLB	O2-C2-C3	-18.80	85.93	109.41
2	A	1	SLB	O2-C2-C3	-18.76	85.99	109.41
2	A	911	SLB	O2-C2-C3	-18.18	86.70	109.41
3	C	914	SLB	O2-C2-C3	-17.97	86.97	109.41
2	C	911	SLB	O2-C2-C3	-17.83	87.14	109.41
2	B	1	SLB	O2-C2-C3	-17.28	87.83	109.41
2	B	911	SLB	O2-C2-O6	-16.16	83.85	110.22
2	B	911	SLB	O2-C2-C3	-16.10	89.31	109.41
2	A	911	SLB	O2-C2-O6	-15.44	85.02	110.22
3	C	914	SLB	O2-C2-O6	-15.03	85.70	110.22
3	B	914	SLB	O2-C2-O6	-14.99	85.77	110.22
3	A	914	SLB	O2-C2-O6	-14.66	86.29	110.22
2	C	911	SLB	O2-C2-O6	-13.90	87.54	110.22
2	B	1	SLB	O2-C2-O6	-12.08	90.51	110.22
2	A	1	SLB	O2-C2-O6	-10.16	93.64	110.22
2	C	1	SLB	O2-C2-O6	-8.79	95.88	110.22
2	C	1	SLB	O10-C10-N5	-3.54	114.65	121.86
3	C	915	SIA	C6-C5-N5	-3.25	105.41	111.07
2	A	912	SIA	C6-C5-N5	-3.22	105.46	111.07
2	B	911	SLB	C6-C5-N5	-3.21	105.48	111.07
2	C	913	SIA	C6-C5-N5	-3.01	105.83	111.07
2	A	2	SIA	C3-C4-C5	-2.95	108.19	111.47
2	A	913	SIA	C6-C5-N5	-2.94	105.95	111.07
2	B	912	SIA	C6-C5-N5	-2.90	106.02	111.07
3	B	915	SIA	C6-C5-N5	-2.86	106.09	111.07
2	B	913	SIA	C4-C5-N5	-2.83	104.27	110.41
3	A	915	SIA	C6-C5-N5	-2.82	106.15	111.07
2	C	912	SIA	C6-C5-N5	-2.81	106.17	111.07
2	A	912	SIA	C4-C5-N5	-2.71	104.51	110.41
2	C	2	SIA	C4-C5-N5	-2.67	104.61	110.41
2	C	3	SIA	C6-C5-N5	-2.63	106.50	111.07
2	A	2	SIA	C6-C5-N5	-2.62	106.50	111.07
3	A	914	SLB	C7-C6-C5	-2.61	110.37	114.32
2	A	913	SIA	C4-C5-N5	-2.60	104.76	110.41
2	B	2	SIA	C4-C5-N5	-2.57	104.82	110.41
2	B	912	SIA	C4-C5-N5	-2.56	104.84	110.41
2	A	3	SIA	C4-C5-N5	-2.56	104.85	110.41
3	B	914	SLB	C7-C6-C5	-2.54	110.48	114.32
2	C	3	SIA	C4-C5-N5	-2.38	105.23	110.41
2	B	3	SIA	C6-C5-N5	-2.38	106.93	111.07
2	C	1	SLB	O7-C7-C6	-2.33	104.05	109.43
2	B	3	SIA	C4-C5-N5	-2.22	105.59	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3	SIA	C6-C5-N5	-2.20	107.23	111.07
2	C	2	SIA	C6-C5-N5	-2.09	107.43	111.07
2	C	913	SIA	C4-C5-N5	-2.07	105.92	110.41
3	C	915	SIA	C4-C5-N5	-2.01	106.03	110.41
2	B	913	SIA	C6-C5-N5	-2.01	107.58	111.07
2	A	911	SLB	O6-C6-C7	2.01	110.30	107.26
2	B	1	SLB	C5-N5-C10	2.11	128.51	123.10
3	B	914	SLB	O6-C6-C7	2.33	110.78	107.26
2	C	1	SLB	O10-C10-C11	2.35	126.38	122.06
2	A	1	SLB	O9-C9-C8	2.88	117.37	111.10
2	A	1	SLB	C6-C5-N5	2.96	116.23	111.07
2	B	911	SLB	O6-C6-C7	3.04	111.86	107.26
2	A	1	SLB	C5-N5-C10	3.09	131.03	123.10
2	C	1	SLB	C5-N5-C10	3.57	132.27	123.10
2	C	1	SLB	O8-C8-C9	3.59	117.60	109.22
2	C	1	SLB	O9-C9-C8	3.91	119.60	111.10
2	C	1	SLB	C4-C5-N5	8.97	129.89	110.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	SLB	3	0
3	A	914	SLB	2	0
2	B	1	SLB	2	0
3	B	914	SLB	1	0
2	C	1	SLB	3	0
2	C	2	SIA	1	0
2	C	911	SLB	1	0

5.6 Ligand geometry [i](#)

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.

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	644/670 (96%)	-0.11	20 (3%)	52 48	12, 19, 41, 53	0
1	B	666/670 (99%)	-0.25	15 (2%)	64 61	12, 18, 31, 44	0
1	C	666/670 (99%)	-0.23	12 (1%)	71 69	11, 19, 34, 49	0
All	All	1976/2010 (98%)	-0.19	47 (2%)	62 59	11, 19, 38, 53	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	VAL	7.8
1	B	245	SER	5.1
1	A	436	ALA	4.6
1	B	910[A]	THR	4.6
1	B	251	VAL	4.5
1	C	245	SER	4.4
1	A	267	VAL	4.3
1	C	269	GLN	4.3
1	A	494	LEU	4.2
1	A	437	ALA	4.1
1	A	491	THR	3.9
1	C	251	VAL	3.9
1	A	438	ASN	3.9
1	C	682	ASP	3.8
1	A	492	SER	3.8
1	B	682	ASP	3.7
1	C	264	ASP	3.6
1	B	269	GLN	3.5
1	B	260	SER	3.5
1	A	439	GLN	3.3
1	B	270	LYS	3.2
1	A	490	GLN	3.1
1	C	256	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	441	TYR	3.0
1	A	503	MET	2.9
1	B	268	GLY	2.9
1	B	264	ASP	2.9
1	B	909	VAL	2.9
1	C	260	SER	2.8
1	C	247	LYS	2.8
1	B	265	THR	2.8
1	A	428[A]	HIS	2.7
1	A	547	ALA	2.6
1	A	268	GLY	2.5
1	A	504	GLY	2.5
1	A	487	PRO	2.5
1	C	681	ASP	2.5
1	A	489	GLN	2.4
1	A	482	PHE	2.4
1	C	266	PRO	2.3
1	A	430	THR	2.3
1	A	440	ARG	2.3
1	B	439[A]	GLN	2.2
1	B	504	GLY	2.2
1	B	487	PRO	2.1
1	B	310	GLU	2.0
1	C	263	ASN	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](#)

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	SLB	B	1	21/21	0.72	0.23	14.20	30,39,40,42	0
2	SLB	A	1	21/21	0.73	0.23	10.83	38,46,48,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SLB	C	1	21/21	0.71	0.24	10.15	39,48,50,51	0
3	SLB	C	914	21/21	0.80	0.19	6.92	24,29,35,38	0
3	SLB	B	914	21/21	0.79	0.28	6.85	29,35,39,40	2
2	SIA	C	2	20/21	0.90	0.14	5.98	30,32,34,35	0
3	SLB	A	914	21/21	0.52	0.34	5.39	29,33,34,34	21
3	SIA	B	915	20/21	0.88	0.13	2.27	17,22,29,31	0
2	SLB	B	911	21/21	0.87	0.14	2.15	26,29,32,32	0
3	SIA	A	915	20/21	0.84	0.16	1.89	22,27,33,34	0
2	SIA	C	3	20/21	0.86	0.14	1.83	28,30,32,33	0
2	SLB	A	911	21/21	0.67	0.23	1.63	51,53,55,56	0
2	SIA	C	912	20/21	0.93	0.10	0.76	19,20,31,31	0
2	SIA	A	2	20/21	0.78	0.15	0.72	30,33,35,35	0
2	SIA	B	912	20/21	0.94	0.10	0.64	24,26,32,33	0
2	SLB	C	911	21/21	0.92	0.10	0.41	19,22,25,27	0
2	SIA	B	3	20/21	0.92	0.12	0.29	21,24,27,28	0
3	SIA	C	915	20/21	0.94	0.10	0.20	15,17,22,25	0
2	SIA	B	2	20/21	0.93	0.10	0.17	24,25,25,27	0
2	SIA	A	912	20/21	0.87	0.14	0.16	46,48,51,52	0
2	SIA	A	3	20/21	0.90	0.12	-0.11	26,29,33,35	0
2	SIA	B	913	20/21	0.86	0.23	-	38,41,43,44	0
2	SIA	A	913	20/21	0.73	0.36	-	56,58,59,59	0
2	SIA	C	913	20/21	0.74	0.27	-	38,41,43,44	0

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(\AA^2)	Q<0.9
4	NA	A	916	1/1	0.99	0.08	-0.19	14,14,14,14	0
4	NA	C	916	1/1	0.98	0.07	-0.49	17,17,17,17	0
4	NA	B	916	1/1	0.99	0.06	-1.33	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.