wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 11:52 AM EDT

PDB ID	:	3KJ4
Title	:	Structure of rat Nogo receptor bound to 1D9 antagonist antibody
Authors	:	Silvian, L.F.
Deposited on	:	2009-11-02
Resolution	:	3.10 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
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 (1)) were used in the production of this report:

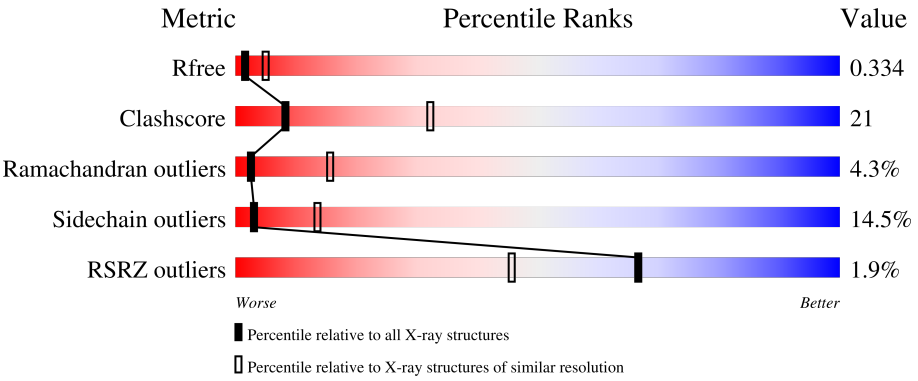
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	B	219	3% 55% 34% 11%
1	L	219	3% 57% 37% 6%
2	C	220	% 45% 40% 13% .
2	H	220	3% 52% 37% 8% .
3	A	286	% 66% 29% . .

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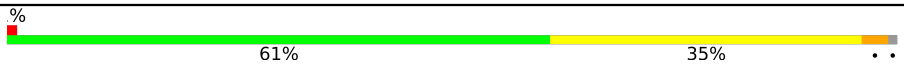
Mol	Chain	Length	Quality of chain
3	D	286	

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
4	MAN	H	303	-	-	-	X
6	NDG	A	313	-	-	X	-
6	NDG	A	314	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11146 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 Fab fragment 1D9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1691	1051	283	348	9			
1	B	219	Total	C	N	O	S	0	0	0
			1697	1054	286	348	9			

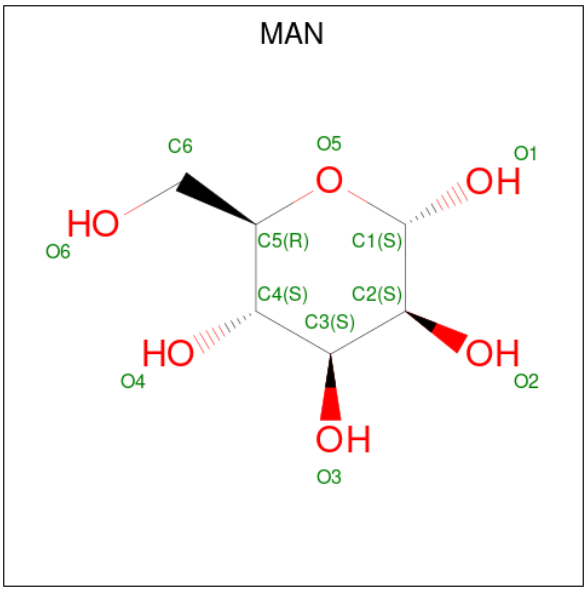
- Molecule 2 is a protein called Fab fragment 1D9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1628	1034	270	317	7			
2	C	216	Total	C	N	O	S	0	0	0
			1621	1029	269	316	7			

- Molecule 3 is a protein called Reticulon-4 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	283	Total	C	N	O	S	0	0	0
			2205	1396	409	388	12			
3	D	283	Total	C	N	O	S	0	0	0
			2207	1398	407	390	12			

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

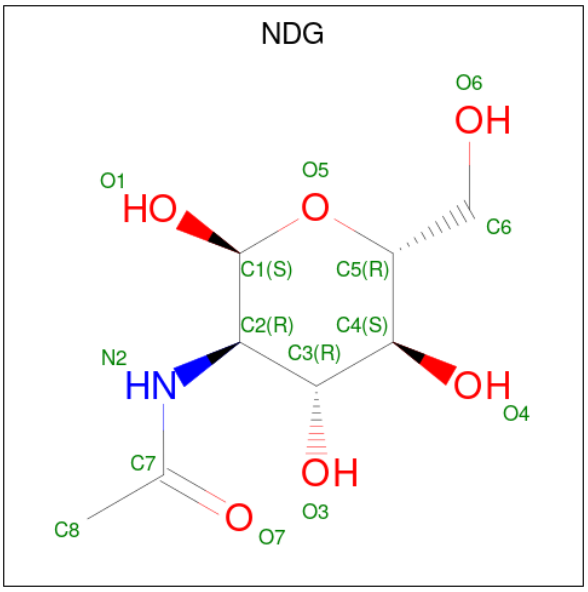


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 11 6 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

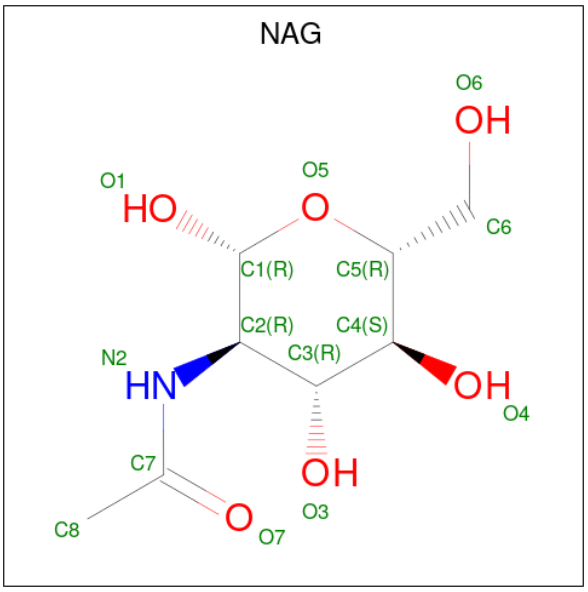
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



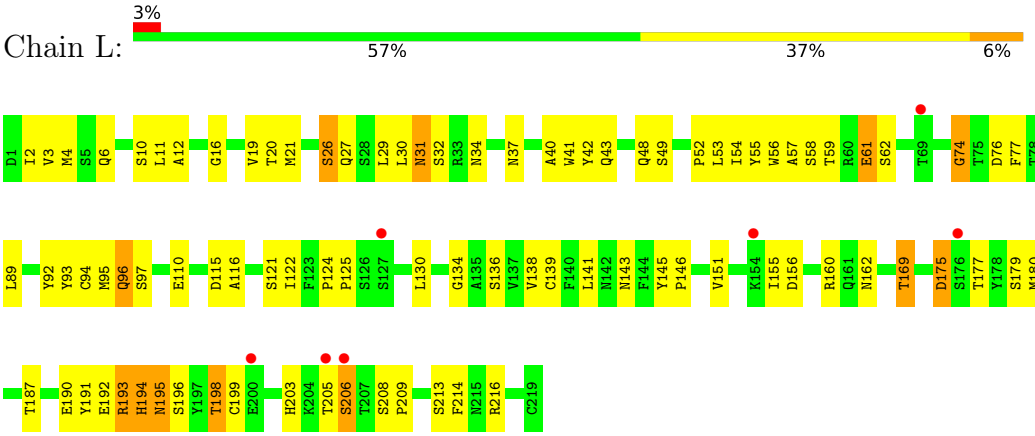
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

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.

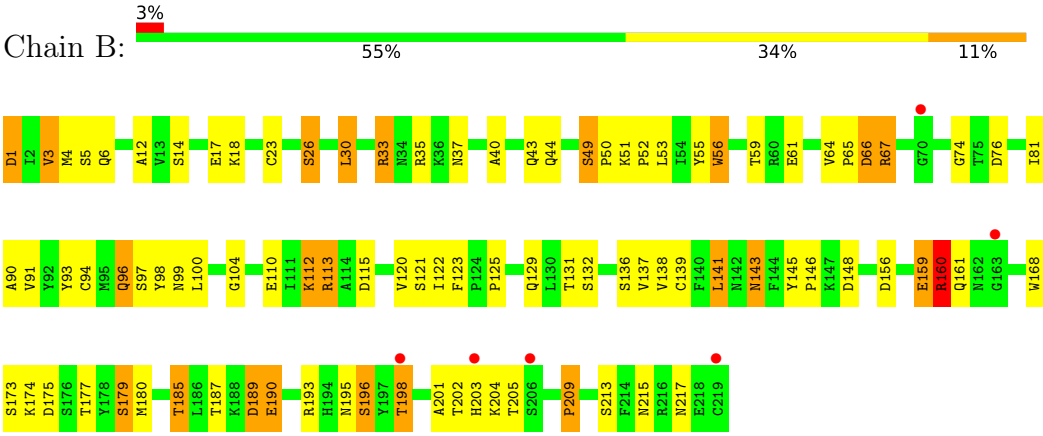
• Molecule 1: Fab fragment 1D9 light chain

Chain L:



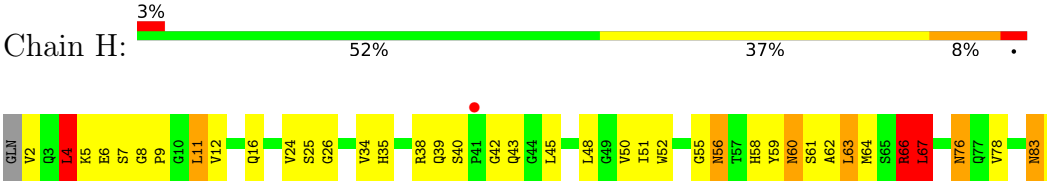
• Molecule 1: Fab fragment 1D9 light chain

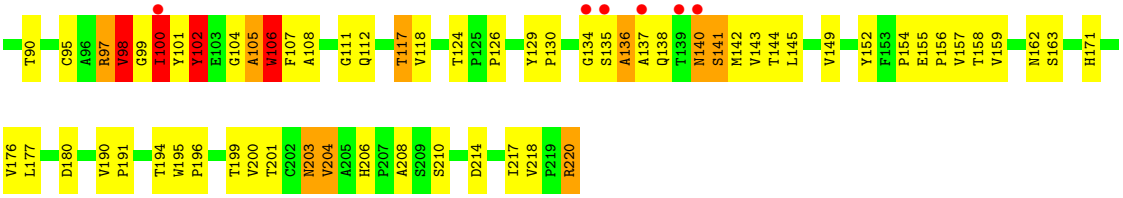
Chain B:



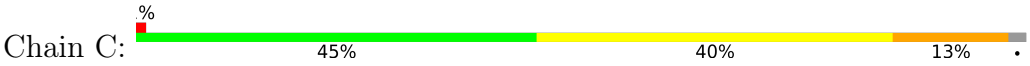
• Molecule 2: Fab fragment 1D9 heavy chain

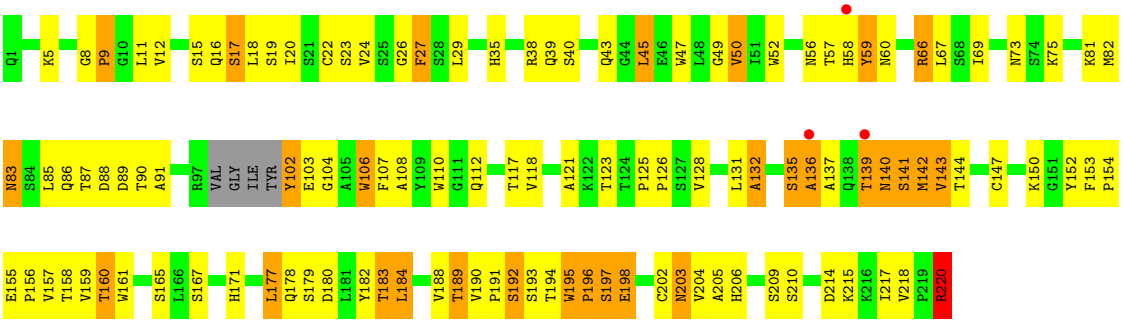
Chain H:



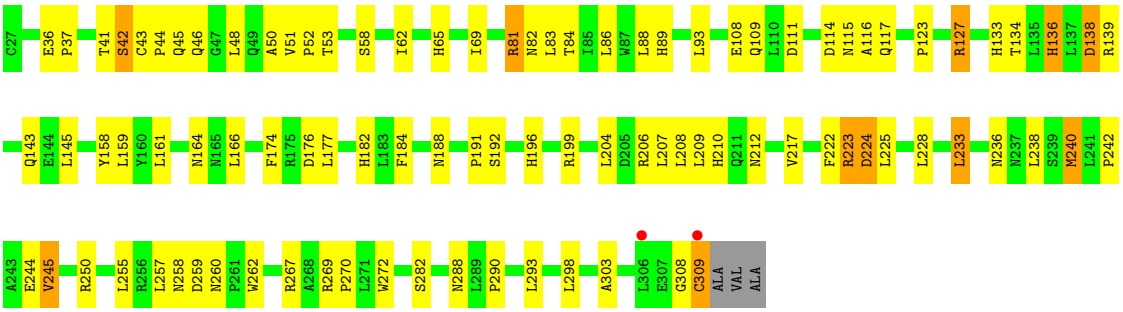


• Molecule 2: Fab fragment 1D9 heavy chain

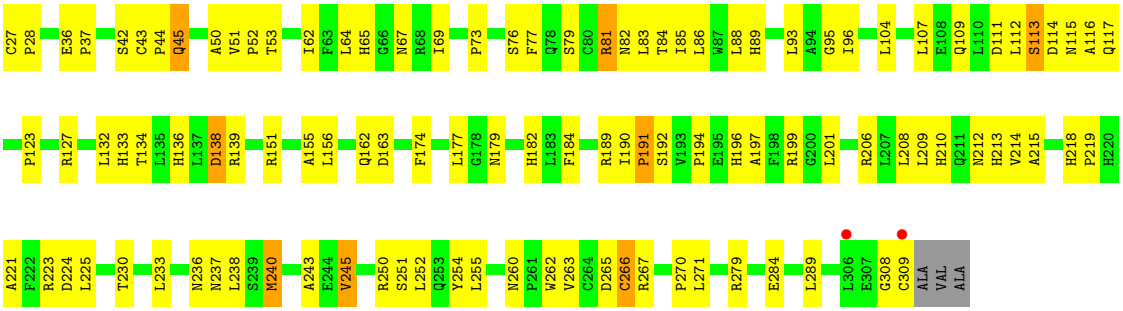




• Molecule 3: Reticulon-4 receptor



• Molecule 3: Reticulon-4 receptor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	188.66Å 125.49Å 90.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.04 – 3.10 44.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.04-3.10) 99.2 (44.04-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.253 , 0.318 0.261 , 0.334	Depositor DCC
R_{free} test set	1987 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	77.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11146	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5129e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, ZN, NDG, 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	B	0.72	1/1734 (0.1%)	0.83	1/2351 (0.0%)
1	L	0.65	0/1728	0.75	1/2344 (0.0%)
2	C	0.67	2/1665 (0.1%)	0.93	3/2277 (0.1%)
2	H	0.65	0/1673	0.84	3/2293 (0.1%)
3	A	0.59	0/2260	0.77	0/3082
3	D	0.58	0/2262	0.74	0/3084
All	All	0.64	3/11322 (0.0%)	0.81	8/15431 (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
2	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	198	GLU	CG-CD	7.41	1.63	1.51
1	B	143	ASN	CB-CG	6.27	1.65	1.51
2	C	198	GLU	CB-CG	5.45	1.62	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	220	ARG	CA-C-O	19.36	160.75	120.10
2	H	4	LEU	CA-CB-CG	7.01	131.41	115.30
2	C	184	LEU	CA-CB-CG	6.44	130.12	115.30
2	H	85	LEU	CA-CB-CG	5.38	127.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	45	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	100	ILE	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	B	1697	0	1627	84	0
1	L	1691	0	1614	71	0
2	C	1621	0	1582	79	0
2	H	1628	0	1577	109	0
3	A	2205	0	2180	64	0
3	D	2207	0	2184	66	0
4	H	11	0	10	0	0
5	C	1	0	0	0	0
5	H	1	0	0	0	0
6	A	28	0	24	9	0
6	D	28	0	24	3	0
7	A	14	0	13	0	0
7	D	14	0	13	1	0
All	All	11146	0	10848	462	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 21.

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)
3:A:82:ASN:HD21	6:A:313:NDG:C1	1.25	1.46
2:H:52:TRP:HE1	2:H:100:ILE:HG13	1.05	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:ASN:ND2	6:A:313:NDG:C1	2.05	1.20
2:H:35:HIS:NE2	2:H:100:ILE:HD11	1.59	1.18
1:B:3:VAL:H	1:B:26:SER:HB3	1.10	1.16

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	B	217/219 (99%)	173 (80%)	33 (15%)	11 (5%)	2 13
1	L	217/219 (99%)	185 (85%)	27 (12%)	5 (2%)	6 28
2	C	212/220 (96%)	175 (82%)	25 (12%)	12 (6%)	1 10
2	H	217/220 (99%)	175 (81%)	26 (12%)	16 (7%)	1 6
3	A	281/286 (98%)	227 (81%)	45 (16%)	9 (3%)	4 22
3	D	281/286 (98%)	230 (82%)	43 (15%)	8 (3%)	5 25
All	All	1425/1450 (98%)	1165 (82%)	199 (14%)	61 (4%)	2 16

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	194	HIS
2	H	67	LEU
2	H	100	ILE
2	H	135	SER
3	A	116	ALA

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 analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	195/196 (100%)	161 (83%)	34 (17%)	2 9
1	L	194/196 (99%)	164 (84%)	30 (16%)	2 11
2	C	184/188 (98%)	142 (77%)	42 (23%)	1 3
2	H	183/188 (97%)	148 (81%)	35 (19%)	1 6
3	A	237/241 (98%)	215 (91%)	22 (9%)	9 32
3	D	238/241 (99%)	222 (93%)	16 (7%)	16 46
All	All	1231/1250 (98%)	1052 (86%)	179 (14%)	3 13

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	169	THR
2	C	128	VAL
1	B	198	THR
2	C	56	ASN
2	C	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	GLN
2	C	112	GLN
1	B	129	GLN
1	B	217	ASN
2	C	206	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
6	NDG	A	314	-	14,14,15	1.33	2 (14%)	17,19,21	2.77	10 (58%)
7	NAG	D	405	-	14,14,15	1.08	1 (7%)	17,19,21	1.73	4 (23%)
7	NAG	A	315	-	14,14,15	0.94	0	17,19,21	3.32	12 (70%)
4	MAN	H	303	-	11,11,12	1.44	2 (18%)	15,15,17	2.34	6 (40%)
6	NDG	D	402	-	14,14,15	1.08	1 (7%)	17,19,21	1.52	4 (23%)
6	NDG	A	313	-	14,14,15	0.71	0	17,19,21	1.93	5 (29%)
6	NDG	D	401	-	14,14,15	0.76	0	17,19,21	2.06	4 (23%)

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
6	NDG	A	314	-	-	2/6/23/26	0/1/1/1
7	NAG	D	405	-	-	4/6/23/26	0/1/1/1
7	NAG	A	315	-	-	3/6/23/26	0/1/1/1
4	MAN	H	303	-	-	1/2/19/22	0/1/1/1
6	NDG	D	402	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	A	313	-	-	2/6/23/26	0/1/1/1
6	NDG	D	401	-	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	303	MAN	C2-C3	3.18	1.57	1.52
6	A	314	NDG	C1-C2	2.51	1.56	1.52
6	D	402	NDG	O5-C1	2.46	1.47	1.43
6	A	314	NDG	C7-N2	2.25	1.42	1.34
7	D	405	NAG	C1-C2	2.24	1.55	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	315	NAG	C1-O5-C5	8.07	123.13	112.19
6	A	314	NDG	O5-C5-C6	5.27	115.46	107.20
7	A	315	NAG	C8-C7-N2	5.00	124.56	116.10
4	H	303	MAN	C1-C2-C3	4.73	115.48	109.67
6	A	313	NDG	O7-C7-N2	4.52	130.26	121.95

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	314	NDG	C8-C7-N2-C2
6	A	314	NDG	O7-C7-N2-C2
6	D	401	NDG	O7-C7-N2-C2
6	D	402	NDG	C8-C7-N2-C2
6	D	402	NDG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	314	NDG	3	0
7	D	405	NAG	1	0
6	D	402	NDG	1	0
6	A	313	NDG	9	0
6	D	401	NDG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	219/219 (100%)	-0.04	6 (2%)	54	31	2, 16, 22, 53	0
1	L	219/219 (100%)	0.03	7 (3%)	47	25	9, 19, 23, 27	0
2	C	216/220 (98%)	-0.23	3 (1%)	75	56	5, 15, 21, 26	0
2	H	219/220 (99%)	-0.16	7 (3%)	47	25	4, 16, 24, 29	0
3	A	283/286 (98%)	-0.21	2 (0%)	87	75	11, 19, 24, 28	0
3	D	283/286 (98%)	-0.17	2 (0%)	87	75	13, 19, 23, 28	0
All	All	1439/1450 (99%)	-0.13	27 (1%)	66	46	2, 18, 23, 53	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	CYS	4.8
1	L	206	SER	4.0
1	B	206	SER	3.6
3	A	309	CYS	3.2
1	L	205	THR	3.2

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

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
4	MAN	H	303	11/12	0.66	0.55	73,75,76,76	0
6	NDG	A	314	14/15	0.73	0.41	74,82,84,84	0
7	NAG	A	315	14/15	0.77	0.22	56,65,70,71	0
6	NDG	D	402	14/15	0.84	0.31	63,66,71,74	0
7	NAG	D	405	14/15	0.85	0.28	71,77,83,85	0
6	NDG	D	401	14/15	0.87	0.14	53,61,73,74	0
6	NDG	A	313	14/15	0.94	0.12	52,60,62,63	0
5	ZN	C	221	1/1	0.97	0.07	64,64,64,64	0
5	ZN	H	221	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.