



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 10:07 am BST

PDB ID : 8S72 / pdb_00008s72
Title : Crystal structure of neutralizing Fab Eq4.Dp46-3D from equine antivenom bound to a consensus short chain three finger alpha-neurotoxin.
Authors : Ayres, F.; Wibmer, C.K.
Deposited on : 2024-02-28
Resolution : 2.78 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

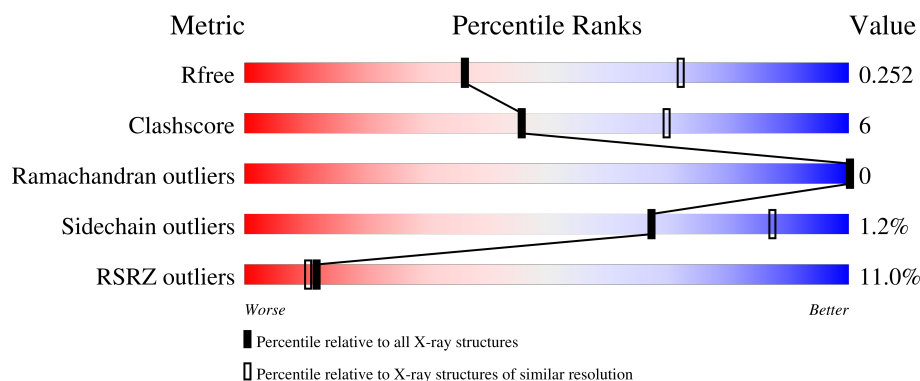
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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 $\leq 5\%$. 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	64	<div> <div>9%</div> <div>89% 11%</div> </div>
1	N	64	<div> <div>6%</div> <div>92% 8%</div> </div>
2	H	233	<div> <div>5%</div> <div>85% 12% .</div> </div>
2	X	233	<div> <div>13%</div> <div>76% 17% 6%</div> </div>
3	L	217	<div> <div>2%</div> <div>89% 11%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	217	<div><div></div><div>25%</div><div>86%</div><div>12%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14484 atoms, of which 6972 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 Short neurotoxin 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	N	64	Total	C	H	N	O	S	0	1	0
			964	297	473	93	92	9			
1	A	64	Total	C	H	N	O	S	0	0	0
			969	295	479	94	92	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-3	GLY	-	expression tag	UNP P01426
N	-2	PRO	-	expression tag	UNP P01426
N	-1	GLY	-	linker	UNP P01426
N	0	GLY	-	linker	UNP P01426
N	1	MET	LEU	conflict	UNP P01426
N	2	ILE	GLU	conflict	UNP P01426
N	4	TYR	HIS	engineered mutation	UNP P01426
N	?	-	PRO	deletion	UNP P01426
N	18	SER	GLY	engineered mutation	UNP P01426
N	21	SER	ASN	engineered mutation	UNP P01426
N	26	THR	VAL	engineered mutation	UNP P01426
N	43	LYS	THR	engineered mutation	UNP P01426
N	51	HIS	ASN	engineered mutation	UNP P01426
N	54	ARG	THR	engineered mutation	UNP P01426
A	-3	GLY	-	expression tag	UNP P01426
A	-2	PRO	-	expression tag	UNP P01426
A	-1	GLY	-	linker	UNP P01426
A	0	GLY	-	linker	UNP P01426
A	1	MET	LEU	conflict	UNP P01426
A	2	ILE	GLU	conflict	UNP P01426
A	4	TYR	HIS	engineered mutation	UNP P01426
A	?	-	PRO	deletion	UNP P01426
A	18	SER	GLY	engineered mutation	UNP P01426
A	21	SER	ASN	engineered mutation	UNP P01426
A	26	THR	VAL	engineered mutation	UNP P01426

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Chain	Residue	Modelled	Actual	Comment	Reference
A	43	LYS	THR	engineered mutation	UNP P01426
A	51	HIS	ASN	engineered mutation	UNP P01426
A	54	ARG	THR	engineered mutation	UNP P01426

- Molecule 2 is a protein called Heavy chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D..

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	218	Total	C	H	N	O	S	0	0	0
			3174	1017	1572	261	319	5			
2	H	226	Total	C	H	N	O	S	0	0	0
			3302	1053	1638	273	332	6			

- Molecule 3 is a protein called Light chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D..

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Y	213	Total	C	H	N	O	S	0	0	0
			2748	906	1281	242	315	4			
3	L	216	Total	C	H	N	O	S	0	0	0
			3123	985	1529	268	336	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	20	Total	O	0	0
			20	20		
4	A	15	Total	O	0	0
			15	15		
4	X	12	Total	O	0	0
			12	12		
4	Y	12	Total	O	0	0
			12	12		
4	H	73	Total	O	0	0
			73	73		
4	L	72	Total	O	0	0
			72	72		

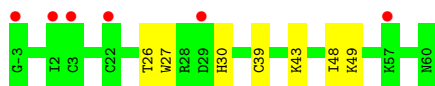
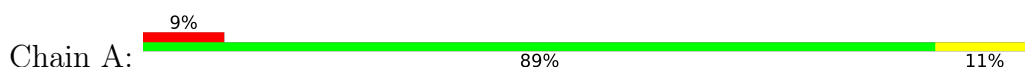
3 Residue-property plots [i](#)

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.

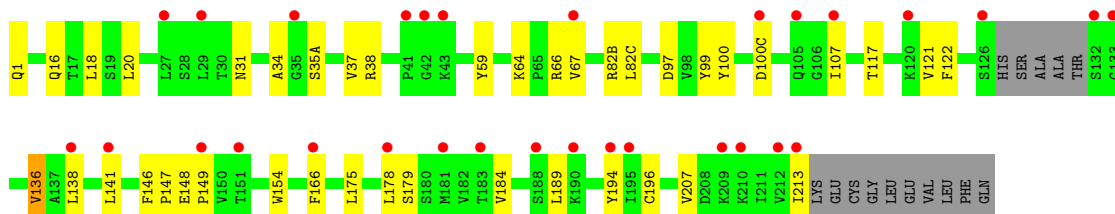
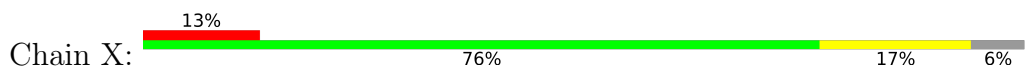
- Molecule 1: Short neurotoxin 1



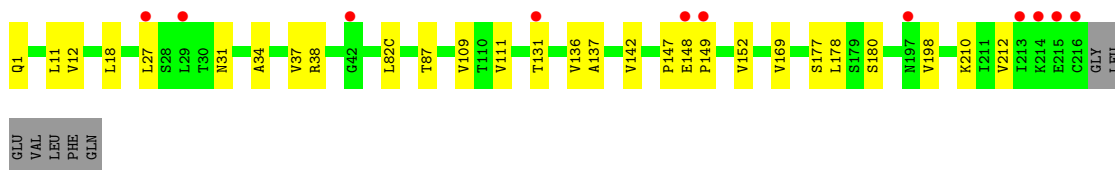
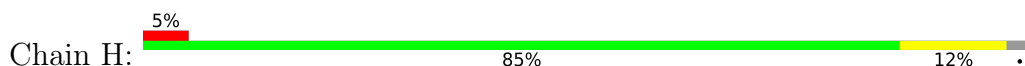
- Molecule 1: Short neurotoxin 1



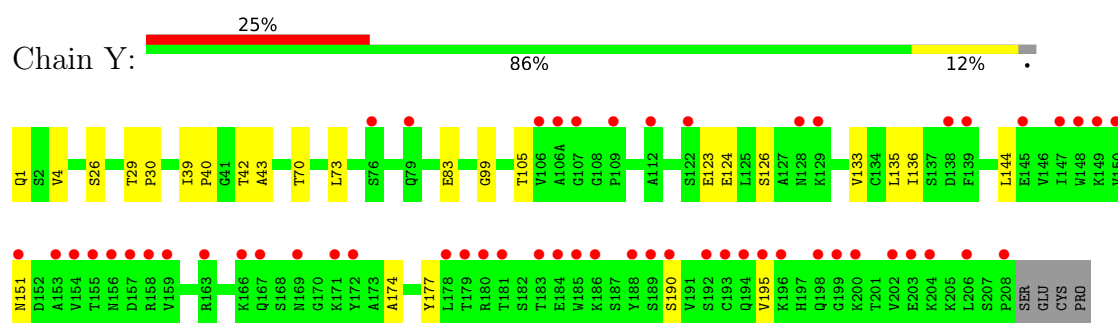
- Molecule 2: Heavy chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D.



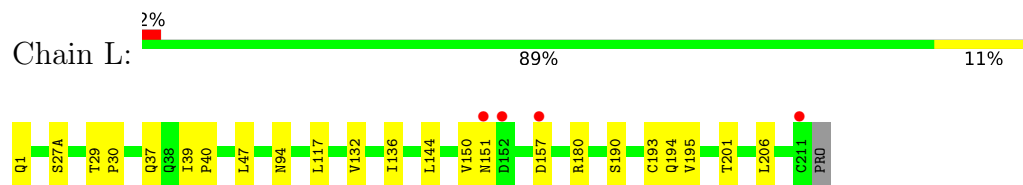
- Molecule 2: Heavy chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D.



- Molecule 3: Light chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D.



- Molecule 3: Light chain of Fab domain from antivenom neutralizing antibody Eq4.Dp46-3D.



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	294.85Å 294.85Å 99.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.60 – 2.78 20.60 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.60-2.78) 99.0 (20.60-2.78)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.228 , 0.249 0.230 , 0.252	Depositor DCC
R_{free} test set	1998 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 0.333 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: PCA

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	0.26	0/500	0.57	0/670
1	N	0.26	0/505	0.55	0/678
2	H	0.20	0/1695	0.41	0/2323
2	X	0.29	0/1631	0.52	0/2237
3	L	0.21	0/1621	0.40	0/2212
3	Y	0.35	0/1494	0.55	0/2058
All	All	0.27	0/7446	0.48	0/10178

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

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	490	479	479	5	0
1	N	491	473	475	2	0
2	H	1664	1638	1638	15	0
2	X	1602	1572	1571	30	0
3	L	1594	1529	1529	16	0
3	Y	1467	1281	1281	19	0
4	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	73	0	0	0	0
4	L	72	0	0	0	0
4	N	20	0	0	0	0
4	X	12	0	0	0	0
4	Y	12	0	0	0	0
All	All	7512	6972	6973	82	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 6.

All (82) 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:Y:42:THR:HG22	3:Y:43:ALA:N	2.06	0.69
3:Y:133:VAL:HG12	3:Y:135:LEU:HD13	1.81	0.62
2:H:169:VAL:HG12	2:H:177:SER:O	2.01	0.60
2:X:99:TYR:N	2:X:100(C):ASP:OD2	2.35	0.58
2:H:18:LEU:HD22	2:H:109:VAL:HG11	1.87	0.57
1:A:43:LYS:HA	4:A:104:HOH:O	2.05	0.57
2:X:166:PHE:HE1	3:Y:174:ALA:C	2.13	0.57
3:L:157:ASP:O	3:L:180:ARG:NH2	2.37	0.57
3:L:136:ILE:HG12	3:L:195:VAL:HG21	1.90	0.54
1:N:7:GLN:HG3	1:N:35:ILE:O	2.08	0.53
3:Y:42:THR:CG2	3:Y:43:ALA:N	2.70	0.53
2:X:178:LEU:C	2:X:178:LEU:HD12	2.33	0.53
2:X:138:LEU:C	2:X:138:LEU:HD12	2.34	0.53
2:X:59:TYR:HB3	2:X:67:VAL:HG11	1.91	0.52
2:H:152:VAL:HG11	2:H:180:SER:CB	2.39	0.52
3:L:151:ASN:N	3:L:190:SER:O	2.43	0.52
2:X:178:LEU:HD12	2:X:179:SER:N	2.26	0.51
2:X:117:THR:HG21	2:X:175:LEU:CD2	2.41	0.50
2:X:136:VAL:HG11	2:X:189:LEU:HD21	1.93	0.50
3:Y:123:GLU:O	3:Y:126:SER:HB3	2.11	0.50
2:X:148:GLU:N	2:X:149:PRO:CD	2.75	0.49
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.94	0.49
2:X:18:LEU:HD11	2:X:20:LEU:HD21	1.94	0.49
3:L:117:LEU:HG	3:L:206:LEU:HD12	1.95	0.49
2:X:122:PHE:CD1	3:Y:124:GLU:HB2	2.48	0.49
2:X:122:PHE:HE1	3:Y:124:GLU:HG3	1.77	0.49
2:H:178:LEU:C	2:H:178:LEU:HD12	2.38	0.48
2:X:66:ARG:HD2	2:X:82(B):ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:133:VAL:HG12	3:Y:135:LEU:CD1	2.44	0.47
2:X:213:ILE:HD12	2:X:213:ILE:H	1.80	0.47
2:H:142:VAL:HG22	2:H:198:VAL:HG21	1.95	0.47
2:X:154:TRP:CZ3	2:X:196:CYS:HB3	2.49	0.46
1:A:26:THR:HG22	1:A:49:LYS:HB2	1.97	0.46
1:A:30:HIS:ND1	1:A:30:HIS:N	2.62	0.46
2:H:148:GLU:N	2:H:149:PRO:CD	2.78	0.46
2:X:146:PHE:CD2	2:X:146:PHE:C	2.94	0.46
3:L:117:LEU:HD13	3:L:193:CYS:HB3	1.98	0.46
2:H:210:LYS:HE2	2:H:212:VAL:HG22	1.97	0.46
2:X:100:TYR:N	2:X:100(C):ASP:OD2	2.41	0.46
2:X:64:LYS:HA	2:X:67:VAL:HG12	1.98	0.45
3:Y:151:ASN:N	3:Y:190:SER:O	2.48	0.45
2:H:87:THR:HG1	2:H:111:VAL:H	1.62	0.45
3:L:27(A):SER:HB3	3:L:94:ASN:ND2	2.32	0.45
1:A:43:LYS:HD3	3:L:94:ASN:HA	2.00	0.44
2:X:122:PHE:CE1	3:Y:124:GLU:HB2	2.52	0.44
3:Y:136:ILE:HG12	3:Y:195:VAL:HG21	2.00	0.44
2:H:131:THR:HG23	2:H:137:ALA:HB2	2.00	0.44
3:L:194:GLN:NE2	3:L:201:THR:HG21	2.32	0.44
2:X:141:LEU:HD12	2:X:178:LEU:O	2.17	0.44
3:L:144:LEU:C	3:L:144:LEU:HD12	2.43	0.44
2:X:16:GLN:O	2:X:82(C):LEU:HD12	2.18	0.44
2:X:59:TYR:HB2	2:X:64:LYS:HG3	2.00	0.43
2:X:121:VAL:HG21	2:X:207:VAL:HG11	2.00	0.43
3:Y:29:THR:HA	3:Y:30:PRO:C	2.44	0.43
3:L:136:ILE:N	3:L:136:ILE:HD12	2.32	0.43
3:Y:83:GLU:HG3	3:Y:105:THR:HA	2.00	0.43
2:H:11:LEU:HB2	2:H:147:PRO:HG3	2.01	0.43
3:L:157:ASP:OD1	3:L:180:ARG:NH2	2.51	0.43
3:Y:39:ILE:O	3:Y:40:PRO:C	2.60	0.43
3:Y:177:TYR:CD1	3:Y:177:TYR:N	2.87	0.43
3:L:117:LEU:HD13	3:L:193:CYS:CB	2.48	0.42
3:L:29:THR:HA	3:L:30:PRO:C	2.44	0.42
2:X:184:VAL:HG11	2:X:194:TYR:CE1	2.54	0.42
3:Y:4:VAL:HG23	3:Y:99:GLY:HA2	2.02	0.42
3:Y:136:ILE:HD12	3:Y:136:ILE:H	1.83	0.42
2:X:37:VAL:HG12	2:X:38:ARG:N	2.34	0.42
2:H:18:LEU:CD2	2:H:109:VAL:HG11	2.49	0.42
3:Y:42:THR:HG22	3:Y:43:ALA:H	1.83	0.41
2:X:31:ASN:HB3	2:X:34:ALA:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:144:LEU:HD12	3:Y:144:LEU:C	2.45	0.41
2:H:12:VAL:HG11	2:H:82(C):LEU:CD1	2.50	0.41
3:L:39:ILE:O	3:L:40:PRO:C	2.64	0.41
2:H:37:VAL:HG12	2:H:38:ARG:N	2.35	0.41
2:X:18:LEU:HD11	2:X:20:LEU:CD2	2.50	0.41
3:L:150:VAL:O	3:L:151:ASN:HB2	2.20	0.41
1:A:27:TRP:HB3	1:A:48:ILE:HG13	2.02	0.41
2:X:97:ASP:HB3	2:X:100(C):ASP:OD1	2.20	0.41
2:X:136:VAL:HG11	2:X:189:LEU:HD11	2.03	0.41
1:N:27:TRP:HB3	1:N:48:ILE:HG13	2.03	0.40
2:H:31:ASN:HB3	2:H:34:ALA:HB3	2.03	0.40
2:X:147:PRO:C	2:X:149:PRO:HD2	2.47	0.40
2:H:136:VAL:HG22	2:H:137:ALA:N	2.37	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	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
1	N	63/64 (98%)	61 (97%)	2 (3%)	0	100	100
2	H	224/233 (96%)	218 (97%)	6 (3%)	0	100	100
2	X	214/233 (92%)	207 (97%)	7 (3%)	0	100	100
3	L	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
3	Y	211/217 (97%)	203 (96%)	8 (4%)	0	100	100
All	All	988/1028 (96%)	956 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	57/57 (100%)	56 (98%)	1 (2%)	54	80
1	N	57/57 (100%)	56 (98%)	1 (2%)	54	80
2	H	187/195 (96%)	186 (100%)	1 (0%)	86	95
2	X	179/195 (92%)	176 (98%)	3 (2%)	56	81
3	L	182/183 (100%)	181 (100%)	1 (0%)	86	95
3	Y	149/183 (81%)	146 (98%)	3 (2%)	50	78
All	All	811/870 (93%)	801 (99%)	10 (1%)	67	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	39	CYS
1	A	39	CYS
2	X	35(A)	SER
2	X	107	ILE
2	X	136	VAL
3	Y	26	SER
3	Y	70	THR
3	Y	73	LEU
2	H	27	LEU
3	L	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	164	HIS
2	H	3	GLN
2	H	164	HIS
3	L	103	HIS
3	L	194	GLN
3	L	197	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
3	PCA	L	1	3	7,8,9	2.21	2 (28%)	9,10,12	2.07	4 (44%)
2	PCA	H	1	2	7,8,9	2.23	2 (28%)	9,10,12	2.04	4 (44%)
3	PCA	Y	1	3	7,8,9	2.20	2 (28%)	9,10,12	2.08	5 (55%)
2	PCA	X	1	2	7,8,9	2.18	2 (28%)	9,10,12	2.20	5 (55%)

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	PCA	L	1	3	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1
3	PCA	Y	1	3	-	0/0/11/13	0/1/1/1
2	PCA	X	1	2	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	PCA	CD-N	4.68	1.46	1.34
2	H	1	PCA	CD-N	4.65	1.46	1.34
3	L	1	PCA	CD-N	4.64	1.46	1.34
3	Y	1	PCA	CD-N	4.62	1.46	1.34
2	H	1	PCA	CA-N	3.47	1.50	1.46
3	L	1	PCA	CA-N	3.43	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	1	PCA	CA-N	3.36	1.50	1.46
2	X	1	PCA	CA-N	3.22	1.50	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1	PCA	OE-CD-CG	-3.10	121.36	126.76
2	X	1	PCA	CA-N-CD	-3.08	103.04	113.58
2	H	1	PCA	OE-CD-CG	-3.05	121.44	126.76
3	Y	1	PCA	OE-CD-CG	-3.01	121.51	126.76
3	L	1	PCA	CA-N-CD	-3.00	103.30	113.58
2	H	1	PCA	CA-N-CD	-3.00	103.32	113.58
3	L	1	PCA	OE-CD-CG	-3.00	121.54	126.76
3	Y	1	PCA	CA-N-CD	-2.99	103.34	113.58
2	X	1	PCA	CB-CA-C	-2.78	108.88	112.70
3	L	1	PCA	CB-CA-N	2.73	111.14	103.30
2	X	1	PCA	CB-CA-N	2.71	111.09	103.30
3	Y	1	PCA	CB-CA-N	2.68	110.98	103.30
2	H	1	PCA	CB-CA-N	2.57	110.68	103.30
2	X	1	PCA	CG-CD-N	2.48	114.80	108.39
2	H	1	PCA	CG-CD-N	2.45	114.74	108.39
3	Y	1	PCA	CG-CD-N	2.45	114.73	108.39
3	L	1	PCA	CG-CD-N	2.41	114.64	108.39
3	Y	1	PCA	CB-CA-C	-2.10	109.81	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	64/64 (100%)	0.68	6 (9%) 15 13	49, 69, 89, 107	0
1	N	64/64 (100%)	0.23	4 (6%) 27 23	31, 57, 71, 94	1 (1%)
2	H	225/233 (96%)	0.03	11 (4%) 36 31	39, 58, 85, 108	0
2	X	217/233 (93%)	0.98	30 (13%) 8 7	61, 103, 147, 169	0
3	L	215/217 (99%)	-0.05	4 (1%) 66 60	40, 60, 78, 108	0
3	Y	212/217 (97%)	1.40	55 (25%) 2 2	57, 122, 151, 160	0
All	All	997/1028 (96%)	0.56	110 (11%) 12 10	31, 70, 144, 169	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	157	ASP	8.4
2	X	132	SER	7.7
3	Y	156	ASN	6.3
3	Y	172	TYR	6.2
1	A	-3	GLY	6.1
3	Y	150	VAL	6.0
3	Y	208	PRO	6.0
3	Y	206	LEU	5.7
3	Y	203	GLU	5.7
3	Y	151	ASN	5.6
3	Y	198	GLN	5.3
3	Y	148	TRP	5.3
3	Y	128	ASN	5.2
2	X	213	ILE	5.1
3	L	211	CYS	4.8
3	Y	158	ARG	4.3
2	H	216	CYS	4.3
3	Y	147	ILE	4.3
3	Y	163	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	X	190	LYS	4.2
3	Y	196	LYS	4.2
2	X	126	SER	4.0
3	Y	186	LYS	4.0
2	X	133	GLY	4.0
3	Y	159	VAL	3.9
2	X	151	THR	3.9
2	X	27	LEU	3.9
3	Y	180	ARG	3.9
3	Y	145	GLU	3.8
3	Y	190	SER	3.8
3	Y	169	ASN	3.8
1	A	57	LYS	3.7
3	Y	194	GLN	3.7
3	Y	166	LYS	3.7
3	Y	192	SER	3.7
3	Y	188	TYR	3.7
3	Y	149	LYS	3.6
1	N	51[A]	HIS	3.6
1	A	3	CYS	3.6
2	H	27	LEU	3.6
3	L	151	ASN	3.6
2	X	141	LEU	3.5
3	Y	139	PHE	3.5
3	Y	138	ASP	3.4
2	X	120	LYS	3.4
3	Y	153	ALA	3.4
3	Y	129	LYS	3.3
3	Y	193	CYS	3.3
2	X	138	LEU	3.3
2	X	29	LEU	3.3
3	Y	195	VAL	3.2
3	Y	200	LYS	3.2
3	Y	109	PRO	3.2
2	X	194	TYR	3.2
2	X	35	GLY	3.2
2	X	212	VAL	3.1
1	N	22	CYS	3.1
2	X	195	ILE	3.0
3	Y	178	LEU	3.0
2	H	131	THR	3.0
3	Y	154	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	X	181	MET	2.9
1	A	29	ASP	2.9
2	H	214	LYS	2.9
3	Y	167	GLN	2.9
1	A	2	ILE	2.8
2	X	67	VAL	2.8
3	Y	179	THR	2.8
2	H	149	PRO	2.8
1	N	3	CYS	2.8
3	Y	181	THR	2.8
3	Y	155	THR	2.7
3	Y	184	GLU	2.7
3	Y	189	SER	2.7
2	H	197	ASN	2.7
3	Y	76	SER	2.6
1	A	22	CYS	2.6
2	X	42	GLY	2.6
3	Y	199	GLY	2.5
2	H	215	GLU	2.5
3	Y	106(A)	ALA	2.5
2	X	107	ILE	2.5
2	H	148	GLU	2.4
2	H	213	ILE	2.4
3	Y	171	LYS	2.4
3	Y	185	TRP	2.4
3	Y	204	LYS	2.4
3	Y	122	SER	2.4
1	N	52	CYS	2.4
2	H	42	GLY	2.4
3	L	152	ASP	2.4
2	X	178	LEU	2.3
2	H	29	LEU	2.3
2	X	41	PRO	2.3
2	X	210	LYS	2.3
3	Y	79	GLN	2.3
3	Y	107	GLY	2.3
3	L	157	ASP	2.3
2	X	183	THR	2.2
2	X	149	PRO	2.2
2	X	166	PHE	2.2
2	X	188	SER	2.2
3	Y	183	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	X	43	LYS	2.1
3	Y	106	VAL	2.1
2	X	100(C)	ASP	2.1
3	Y	202	VAL	2.1
2	X	209	LYS	2.0
2	X	105	GLN	2.0
3	Y	112	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å ²)	Q<0.9
2	PCA	X	1	8/9	0.35	0.24	99,111,135,135	0
2	PCA	H	1	8/9	0.49	0.20	77,100,110,122	0
3	PCA	Y	1	8/9	0.88	0.22	67,77,87,89	0
3	PCA	L	1	8/9	0.88	0.15	50,62,69,82	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.