



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 AM UTC

PDB ID : 5VEB / pdb_00005veb
Title : Crystal structure of a Fab binding to extracellular domain 5 of Cadherin-6
Authors : Zhu, X.; Bialucha, C.U.; London, A.; Clark, K.; Hu, T.
Deposited on : 2017-04-04
Resolution : 2.34 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

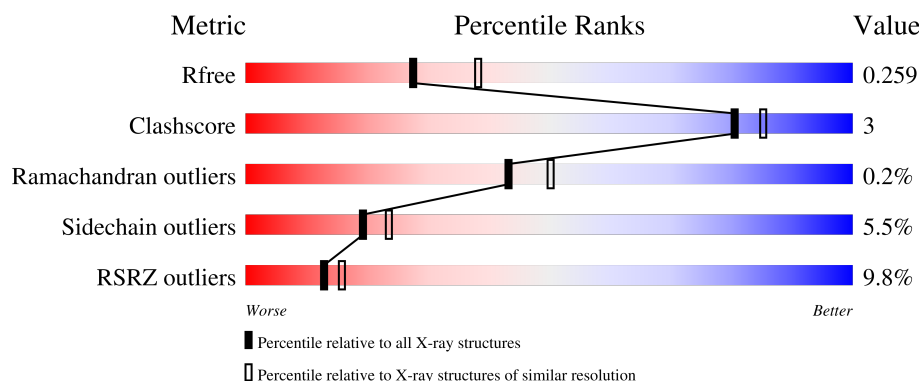
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	225	8% 87% 11% .
2	B	215	7% 91% 8% .
2	L	215	4% 92% 7% .
3	H	225	22% 88% 9% .
4	X	125	8% 71% 13% 16%

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Mol	Chain	Length	Quality of chain
4	Y	125	5% 73% 11% • 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8497 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 anti-CDH6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1640	1026	282	325	7			

- Molecule 2 is a protein called anti-CDH6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1643	1026	274	337	6			
2	L	215	Total	C	N	O	S	0	0	0
			1643	1026	274	337	6			

- Molecule 3 is a protein called anti-CDH6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1633	1022	282	322	7			

- Molecule 4 is a protein called Cadherin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	105	Total	C	N	O	S	0	0	0
			810	506	137	163	4			
4	Y	107	Total	C	N	O	S	0	0	0
			831	520	139	168	4			

There are 12 discrepancies between the modelled and reference sequences:

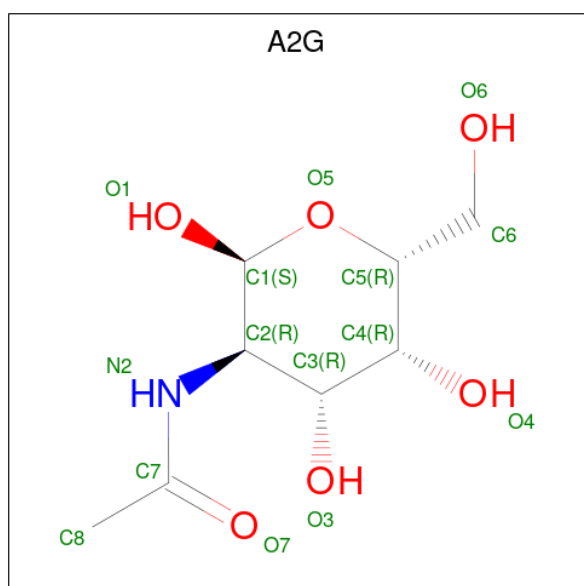
Chain	Residue	Modelled	Actual	Comment	Reference
X	609	LEU	-	expression tag	UNP P55285
X	610	GLU	-	expression tag	UNP P55285
X	611	VAL	-	expression tag	UNP P55285
X	612	LEU	-	expression tag	UNP P55285

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Chain	Residue	Modelled	Actual	Comment	Reference
X	613	PHE	-	expression tag	UNP P55285
X	614	GLN	-	expression tag	UNP P55285
Y	609	LEU	-	expression tag	UNP P55285
Y	610	GLU	-	expression tag	UNP P55285
Y	611	VAL	-	expression tag	UNP P55285
Y	612	LEU	-	expression tag	UNP P55285
Y	613	PHE	-	expression tag	UNP P55285
Y	614	GLN	-	expression tag	UNP P55285

- Molecule 5 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	X	1	Total	C	N	O	0	0
			14	8	1	5		
5	X	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	49	Total	O	0	0
			49	49		

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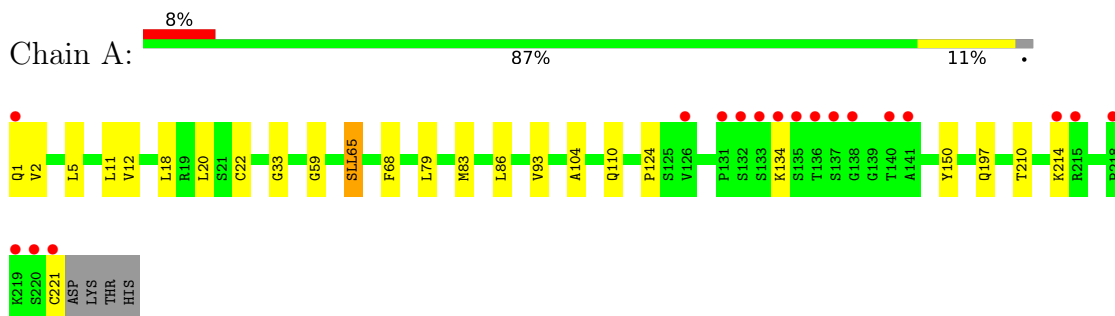
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	64	Total 64	O 64	0	0
6	H	16	Total 16	O 16	0	0
6	L	62	Total 62	O 62	0	0
6	X	24	Total 24	O 24	0	0
6	Y	26	Total 26	O 26	0	0

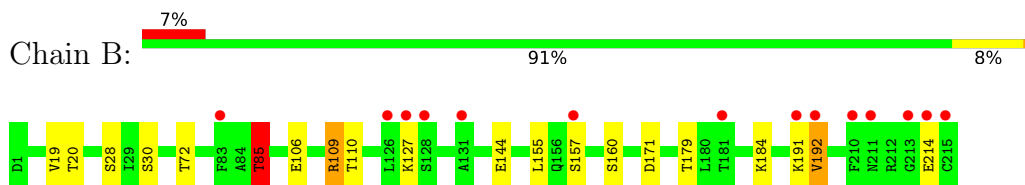
3 Residue-property plots [i](#)

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.

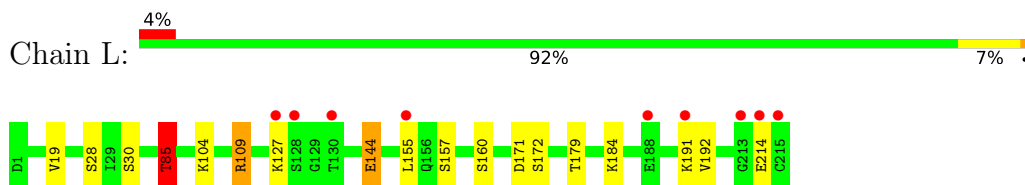
- Molecule 1: anti-CDH6 Fab heavy chain



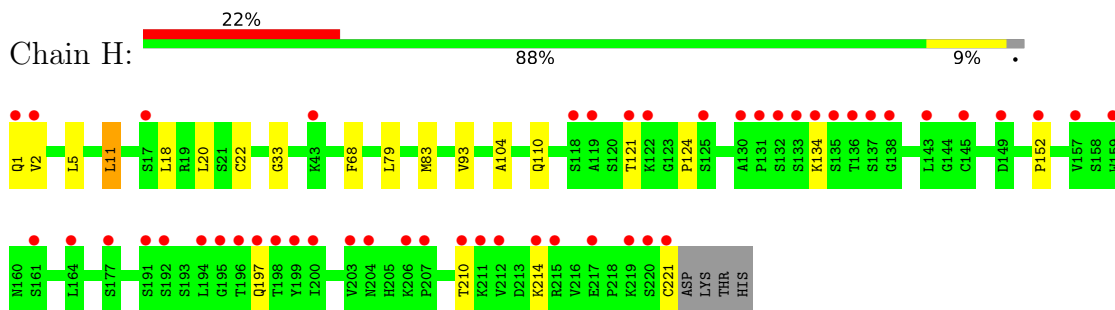
- Molecule 2: anti-CDH6 Fab light chain



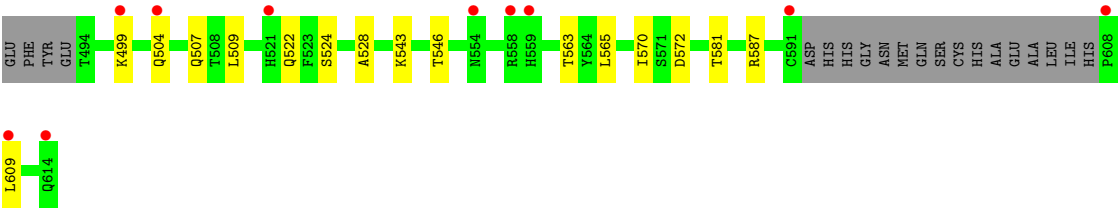
- Molecule 2: anti-CDH6 Fab light chain



- Molecule 3: anti-CDH6 Fab heavy chain



- Molecule 4: Cadherin-6



• Molecule 4: Cadherin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.83Å 88.86Å 186.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.23 – 2.34 80.23 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.1 (80.23-2.34) 99.1 (80.23-2.34)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.34Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.212 , 0.252 0.218 , 0.259	Depositor DCC
R_{free} test set	2824 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8497	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 61.11 % 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 1.3760e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A2G, SLL

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	0.83	0/1662	1.16	4/2261 (0.2%)
2	B	0.86	0/1678	1.16	6/2278 (0.3%)
2	L	0.84	0/1678	1.18	6/2278 (0.3%)
3	H	0.78	0/1672	1.17	4/2275 (0.2%)
4	X	0.81	0/825	1.17	2/1120 (0.2%)
4	Y	0.85	0/847	1.19	2/1150 (0.2%)
All	All	0.83	0/8362	1.17	24/11362 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	171	ASP	CA-CB-CG	8.08	120.68	112.60
3	H	68	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	68	PHE	CA-CB-CG	7.04	120.84	113.80
2	L	85	THR	CB-CA-C	6.52	120.44	109.48
4	X	572	ASP	CA-CB-CG	6.46	119.06	112.60
4	X	570	ILE	N-CA-CB	6.25	119.75	111.25
3	H	33	GLY	N-CA-C	-6.17	103.15	111.54
2	L	109	ARG	N-CA-CB	-6.16	101.64	111.43
1	A	33	GLY	N-CA-C	-6.12	103.22	111.54
4	Y	572	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	93	VAL	N-CA-C	-5.77	100.27	108.58
3	H	93	VAL	N-CA-C	-5.55	100.58	108.58
2	B	85	THR	CB-CA-C	5.52	119.27	109.72
2	B	171	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	85	THR	N-CA-CB	5.48	119.18	110.57
2	B	109	ARG	N-CA-CB	-5.42	103.12	111.46
2	B	184	LYS	CA-C-N	5.41	127.47	120.44
2	B	184	LYS	C-N-CA	5.41	127.47	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ALA	N-CA-C	-5.39	102.54	110.52
3	H	104	ALA	N-CA-C	-5.33	102.63	110.52
2	L	184	LYS	CA-C-N	5.29	127.32	120.44
2	L	184	LYS	C-N-CA	5.29	127.32	120.44
4	Y	515	ASP	CA-CB-CG	5.26	117.86	112.60
2	L	85	THR	N-CA-CB	5.22	119.14	110.52

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	1640	0	1592	8	0
2	B	1643	0	1598	8	0
2	L	1643	0	1598	4	0
3	H	1633	0	1591	6	0
4	X	810	0	776	6	0
4	Y	831	0	791	8	0
5	X	28	0	24	4	0
5	Y	28	0	24	5	0
6	A	49	0	0	0	0
6	B	64	0	0	3	0
6	H	16	0	0	0	0
6	L	62	0	0	1	0
6	X	24	0	0	0	0
6	Y	26	0	0	1	0
All	All	8497	0	7994	42	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 (42) 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)
4:Y:528:ALA:HB1	5:Y:2001:A2G:H14	1.30	1.05
4:X:528:ALA:HB1	5:X:2001:A2G:H14	1.46	0.96
4:Y:528:ALA:CB	5:Y:2001:A2G:H14	2.03	0.87
4:X:528:ALA:CB	5:X:2001:A2G:H14	2.09	0.82
2:B:20:THR:HG23	2:B:72:THR:CG2	2.17	0.74
2:B:20:THR:HG23	2:B:72:THR:HG23	1.69	0.73
5:X:2002:A2G:C1	5:X:2002:A2G:O6	2.50	0.60
4:Y:608:PRO:HG2	6:Y:2122:HOH:O	2.02	0.59
1:A:59:GLY:HA2	1:A:65:SLL:HL	1.87	0.56
4:X:528:ALA:HB1	5:X:2001:A2G:C6	2.29	0.56
4:Y:528:ALA:HB1	5:Y:2001:A2G:C6	2.21	0.56
2:B:20:THR:CG2	2:B:72:THR:HG23	2.37	0.54
2:B:192:VAL:HG12	6:B:332:HOH:O	2.07	0.53
3:H:11:LEU:HG	3:H:152:PRO:HG3	1.90	0.53
2:B:85:THR:HG23	6:B:317:HOH:O	2.08	0.53
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.89	0.53
1:A:22:CYS:HB3	1:A:79:LEU:HB3	1.90	0.52
3:H:124:PRO:HD2	3:H:210:THR:HG21	1.91	0.52
4:Y:557:ASN:HB3	4:Y:560:GLU:HB2	1.92	0.52
1:A:124:PRO:HD2	1:A:210:THR:HG21	1.92	0.51
1:A:12:VAL:HG11	1:A:86:LEU:HD13	1.92	0.51
4:X:563:THR:HG22	4:X:587:ARG:HG2	1.94	0.49
4:X:507:GLN:HG2	4:X:609:LEU:HD22	1.94	0.48
3:H:1:GLN:HG3	3:H:2:VAL:H	1.79	0.47
4:Y:509:LEU:O	4:Y:546:THR:HA	2.16	0.46
5:Y:2002:A2G:C1	5:Y:2002:A2G:H8B	2.45	0.46
3:H:20:LEU:HG	3:H:83:MET:HE2	1.97	0.46
2:L:109:ARG:HG3	2:L:172:SER:HB2	1.99	0.45
4:X:509:LEU:O	4:X:546:THR:HA	2.16	0.45
4:Y:571:SER:HB2	4:Y:579:SER:HB3	1.98	0.45
2:L:85:THR:HG22	2:L:104:LYS:HG3	1.99	0.45
2:B:109:ARG:HD3	2:B:110:THR:O	2.17	0.44
2:B:192:VAL:CG1	6:B:332:HOH:O	2.66	0.44
2:L:144:GLU:HB2	6:L:358:HOH:O	2.17	0.43
1:A:1:GLN:HG3	1:A:2:VAL:H	1.82	0.43
1:A:20:LEU:HG	1:A:83:MET:HE2	1.99	0.43
3:H:18:LEU:HB3	3:H:83:MET:HE3	2.00	0.43
4:Y:579:SER:O	5:Y:2001:A2G:H8B	2.19	0.42
1:A:18:LEU:HB3	1:A:83:MET:HE3	2.02	0.41
1:A:124:PRO:HB3	1:A:150:TYR:HB3	2.02	0.41
2:B:160:SER:HA	2:B:179:THR:O	2.21	0.41
2:L:160:SER:HA	2:L:179:THR:O	2.20	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	218/225 (97%)	215 (99%)	3 (1%)	0	100	100
2	B	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	24	26
2	L	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	24	26
3	H	219/225 (97%)	216 (99%)	3 (1%)	0	100	100
4	X	101/125 (81%)	100 (99%)	1 (1%)	0	100	100
4	Y	103/125 (82%)	101 (98%)	2 (2%)	0	100	100
All	All	1067/1130 (94%)	1042 (98%)	23 (2%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	30	SER
2	B	30	SER

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	A	182/186 (98%)	175 (96%)	7 (4%)	29	38
2	B	190/190 (100%)	179 (94%)	11 (6%)	18	22
2	L	190/190 (100%)	180 (95%)	10 (5%)	20	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	183/187 (98%)	175 (96%)	8 (4%)	25	33
4	X	92/109 (84%)	85 (92%)	7 (8%)	12	13
4	Y	94/109 (86%)	86 (92%)	8 (8%)	10	10
All	All	931/971 (96%)	880 (94%)	51 (6%)	19	23

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	LEU
1	A	110	GLN
1	A	134	LYS
1	A	197	GLN
1	A	214	LYS
1	A	221	CYS
2	B	19	VAL
2	B	28	SER
2	B	85	THR
2	B	106	GLU
2	B	127	LYS
2	B	144	GLU
2	B	155	LEU
2	B	157	SER
2	B	191	LYS
2	B	192	VAL
2	B	214	GLU
3	H	5	LEU
3	H	11	LEU
3	H	110	GLN
3	H	121	THR
3	H	134	LYS
3	H	197	GLN
3	H	214	LYS
3	H	221	CYS
2	L	19	VAL
2	L	28	SER
2	L	85	THR
2	L	127	LYS
2	L	144	GLU
2	L	155	LEU
2	L	157	SER

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Mol	Chain	Res	Type
2	L	191	LYS
2	L	192	VAL
2	L	214	GLU
4	X	499	LYS
4	X	504	GLN
4	X	522	GLN
4	X	524	SER
4	X	543	LYS
4	X	565	LEU
4	X	581	THR
4	Y	504	GLN
4	Y	522	GLN
4	Y	524	SER
4	Y	543	LYS
4	Y	560	GLU
4	Y	565	LEU
4	Y	571	SER
4	Y	581	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	82	GLN
2	B	148	GLN
2	B	161	GLN
2	B	211	ASN
3	H	1	GLN
3	H	169	HIS
2	L	79	GLN
2	L	148	GLN
2	L	211	ASN
4	X	510	HIS
4	X	522	GLN
4	X	536	ASN
4	Y	510	HIS
4	Y	521	HIS
4	Y	522	GLN
4	Y	536	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	SLL	A	65	1	14,15,16	2.57	4 (28%)	12,17,19	5.92	7 (58%)

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
1	SLL	A	65	1	-	5/14/15/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	SLL	OX-CX	6.24	1.35	1.23
1	A	65	SLL	CX-NZ	4.55	1.44	1.33
1	A	65	SLL	OP1-CP	4.01	1.35	1.22
1	A	65	SLL	OP2-CP	-2.99	1.20	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SLL	CE-NZ-CX	16.97	154.42	122.82
1	A	65	SLL	CK-CX-NZ	-6.44	104.60	116.34
1	A	65	SLL	CL-CK-CX	5.57	124.12	112.67
1	A	65	SLL	OX-CX-NZ	-5.53	112.19	123.03
1	A	65	SLL	CK-CL-CP	3.35	122.56	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SLL	OP2-CP-CL	2.73	122.62	114.00
1	A	65	SLL	OX-CX-CK	2.33	126.24	122.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	SLL	CX-CK-CL-CP
1	A	65	SLL	OX-CX-NZ-CE
1	A	65	SLL	CK-CX-NZ-CE
1	A	65	SLL	CD-CE-NZ-CX
1	A	65	SLL	CK-CL-CP-OP1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	SLL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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
5	A2G	X	2001	4	14,14,15	0.85	0	17,19,21	1.25	3 (17%)
5	A2G	X	2002	4	14,14,15	1.33	1 (7%)	17,19,21	3.61	8 (47%)
5	A2G	Y	2002	4	14,14,15	0.80	0	17,19,21	1.10	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	A2G	Y	2001	4	14,14,15	0.82	0	17,19,21	1.44	3 (17%)

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
5	A2G	X	2001	4	-	2/6/23/26	0/1/1/1
5	A2G	X	2002	4	-	3/6/23/26	0/1/1/1
5	A2G	Y	2002	4	-	6/6/23/26	0/1/1/1
5	A2G	Y	2001	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	2002	A2G	C1-C2	3.92	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	2002	A2G	C1-O5-C5	7.15	121.77	112.19
5	X	2002	A2G	O5-C5-C4	-6.47	95.09	110.83
5	X	2002	A2G	C3-C4-C5	6.44	121.90	110.23
5	X	2002	A2G	O3-C3-C2	6.04	121.95	109.40
5	X	2002	A2G	C4-C3-C2	-3.97	105.21	111.02
5	Y	2001	A2G	C2-N2-C7	-3.01	118.86	122.90
5	X	2002	A2G	O7-C7-N2	2.86	127.03	121.98
5	Y	2001	A2G	C1-O5-C5	2.74	115.86	112.19
5	X	2002	A2G	C2-N2-C7	2.71	126.53	122.90
5	X	2001	A2G	C1-O5-C5	2.46	115.48	112.19
5	X	2002	A2G	O5-C1-C2	-2.40	107.58	111.29
5	X	2001	A2G	O7-C7-N2	2.28	126.00	121.98
5	Y	2002	A2G	O7-C7-N2	2.23	125.92	121.98
5	X	2001	A2G	C2-N2-C7	-2.10	120.09	122.90
5	Y	2001	A2G	O7-C7-N2	2.06	125.62	121.98
5	Y	2002	A2G	C2-N2-C7	2.05	125.65	122.90
5	Y	2002	A2G	O7-C7-C8	-2.03	118.44	122.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	2002	A2G	C1-C2-N2-C7
5	X	2001	A2G	O5-C5-C6-O6
5	Y	2001	A2G	O5-C5-C6-O6
5	Y	2002	A2G	O5-C5-C6-O6
5	X	2002	A2G	O5-C5-C6-O6
5	X	2001	A2G	C4-C5-C6-O6
5	Y	2001	A2G	C4-C5-C6-O6
5	Y	2002	A2G	C4-C5-C6-O6
5	X	2002	A2G	C4-C5-C6-O6
5	Y	2002	A2G	O7-C7-N2-C2
5	Y	2002	A2G	C8-C7-N2-C2
5	Y	2002	A2G	C3-C2-N2-C7
5	Y	2002	A2G	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	2001	A2G	3	0
5	X	2002	A2G	1	0
5	Y	2002	A2G	1	0
5	Y	2001	A2G	4	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, 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	220/225 (97%)	0.52	18 (8%)	17 21	16, 36, 79, 114	0
2	B	215/215 (100%)	0.35	14 (6%)	25 29	18, 33, 61, 117	0
2	L	215/215 (100%)	0.39	9 (4%)	40 46	19, 36, 61, 111	0
3	H	221/225 (98%)	1.20	49 (22%)	2 2	18, 46, 81, 118	0
4	X	105/125 (84%)	0.56	10 (9%)	14 17	24, 40, 60, 82	0
4	Y	107/125 (85%)	0.53	6 (5%)	30 35	22, 37, 64, 85	0
All	All	1083/1130 (95%)	0.60	106 (9%)	13 16	16, 38, 72, 118	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	135	SER	10.1
1	A	135	SER	7.0
3	H	137	SER	6.9
3	H	134	LYS	6.3
3	H	138	GLY	5.8
1	A	137	SER	5.8
4	Y	492	TYR	5.4
1	A	136	THR	5.2
3	H	136	THR	5.1
4	Y	608	PRO	4.6
3	H	132	SER	4.4
1	A	134	LYS	4.3
3	H	221	CYS	4.3
1	A	138	GLY	4.1
2	B	215	CYS	4.0
4	X	608	PRO	3.9
4	X	591	CYS	3.8
2	L	127	LYS	3.7
2	L	191	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
3	H	195	GLY	3.7
3	H	1	GLN	3.6
3	H	203	VAL	3.6
3	H	194	LEU	3.6
3	H	133	SER	3.6
2	L	215	CYS	3.5
3	H	219	LYS	3.5
1	A	219	LYS	3.4
1	A	221	CYS	3.4
3	H	198	THR	3.3
1	A	1	GLN	3.3
3	H	157	VAL	3.2
4	Y	614	GLN	3.1
4	Y	591	CYS	3.1
3	H	118	SER	3.0
4	X	559	HIS	3.0
3	H	159	TRP	3.0
1	A	132	SER	3.0
2	B	191	LYS	3.0
1	A	214	LYS	2.9
3	H	17	SER	2.9
3	H	2	VAL	2.9
2	L	213	GLY	2.9
4	Y	558	ARG	2.9
3	H	214	LYS	2.9
3	H	196	THR	2.8
1	A	220	SER	2.8
2	B	157	SER	2.8
2	B	83	PHE	2.7
2	B	126	LEU	2.7
3	H	164	LEU	2.7
4	X	558	ARG	2.6
3	H	212	VAL	2.6
3	H	177	SER	2.6
3	H	200	ILE	2.6
3	H	197	GLN	2.6
3	H	215	ARG	2.6
1	A	141	ALA	2.6
2	B	181	THR	2.6
3	H	207	PRO	2.6
1	A	133	SER	2.6
3	H	145	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
4	X	614	GLN	2.5
3	H	204	ASN	2.5
2	B	210	PHE	2.5
4	Y	493	GLU	2.4
3	H	220	SER	2.4
2	L	214	GLU	2.4
3	H	152	PRO	2.4
3	H	121	THR	2.4
4	X	554	ASN	2.4
3	H	210	THR	2.4
3	H	211	LYS	2.3
4	X	521	HIS	2.3
2	B	211	ASN	2.3
3	H	43	LYS	2.3
3	H	192	SER	2.3
2	L	155	LEU	2.3
2	L	130	THR	2.3
2	B	127	LYS	2.3
4	X	499	LYS	2.3
3	H	149	ASP	2.2
1	A	215	ARG	2.2
2	B	214	GLU	2.2
3	H	119	ALA	2.2
1	A	140	THR	2.2
3	H	161	SER	2.2
3	H	131	PRO	2.2
2	B	131	ALA	2.2
1	A	131	PRO	2.2
2	B	213	GLY	2.2
3	H	199	TYR	2.1
4	X	609	LEU	2.1
1	A	126	VAL	2.1
2	L	128	SER	2.1
3	H	191	SER	2.1
3	H	206	LYS	2.1
2	B	128	SER	2.1
3	H	125	SER	2.1
3	H	130	ALA	2.1
2	L	188	GLU	2.0
3	H	217	GLU	2.0
1	A	218	PRO	2.0
2	B	192	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	122	LYS	2.0
4	X	504	GLN	2.0
3	H	143	LEU	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
1	SLI	A	65	16/17	0.90	0.17	22,42,61,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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
5	A2G	X	2001	14/15	0.76	0.18	54,58,72,76	0
5	A2G	Y	2002	14/15	0.78	0.19	59,63,77,77	0
5	A2G	X	2002	14/15	0.80	0.17	60,64,77,79	0
5	A2G	Y	2001	14/15	0.81	0.18	39,49,60,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.