



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2024 – 05:06 PM EDT

PDB ID : 5VEB
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
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) : 2.36.1

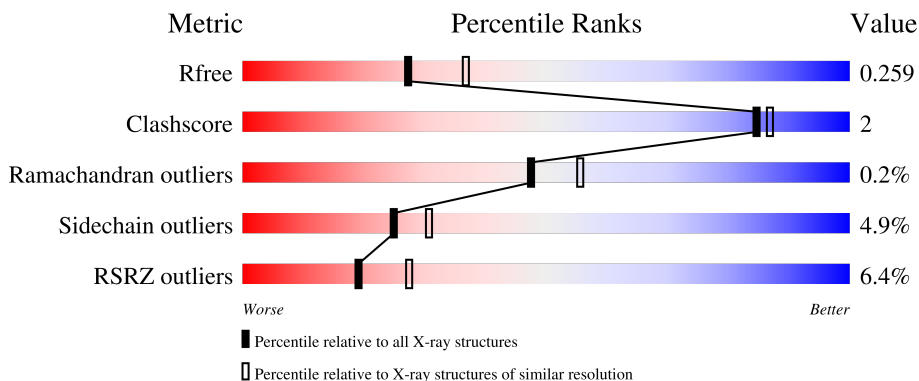
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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.



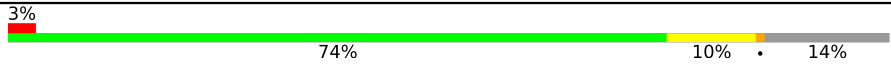
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	 5% 90% 8%
2	B	215	 6% 93% 7%
2	L	215	 5% 93% 6%
3	H	225	 12% 92% 6%
4	X	125	 % 74% 10% 16%

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Mol	Chain	Length	Quality of chain
4	Y	125	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '3%', a large green segment labeled '74%', a yellow segment labeled '10%', and a grey segment at the end labeled '14%'.</p>

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	221	1640	1026	282	325	7	0	0	0

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

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

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

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

- Molecule 4 is a protein called Cadherin-6.

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

There are 12 discrepancies between the modelled and reference sequences:

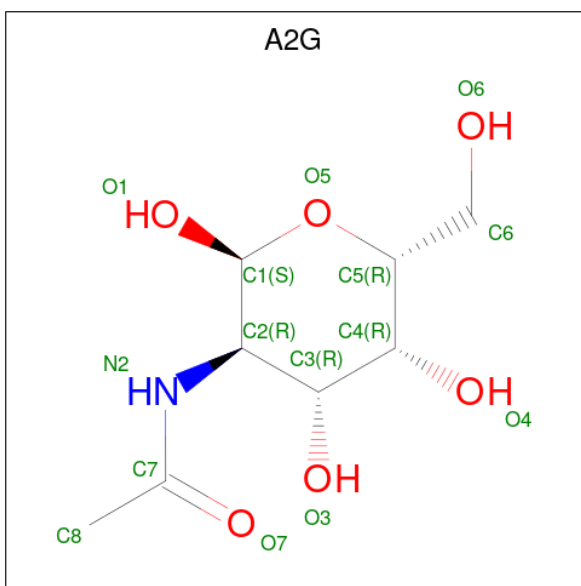
Chain	Residue	Modelled	Actual	Comment	Reference
X	609	LEU	-	expression tag	UNP P55285
X	610	GLU	-	expression tag	UNP P55285
X	611	VAL	-	expression tag	UNP P55285
X	612	LEU	-	expression tag	UNP P55285

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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 (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



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

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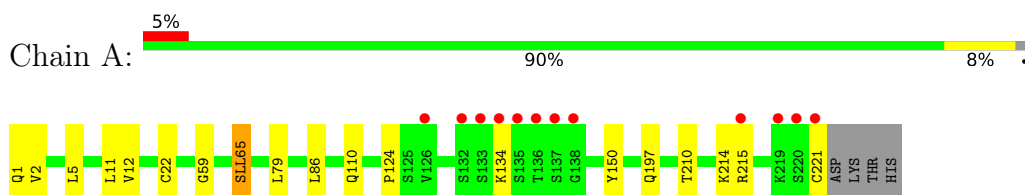
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	64	Total O 64 64	0	0
6	H	16	Total O 16 16	0	0
6	L	62	Total O 62 62	0	0
6	X	24	Total O 24 24	0	0
6	Y	26	Total O 26 26	0	0

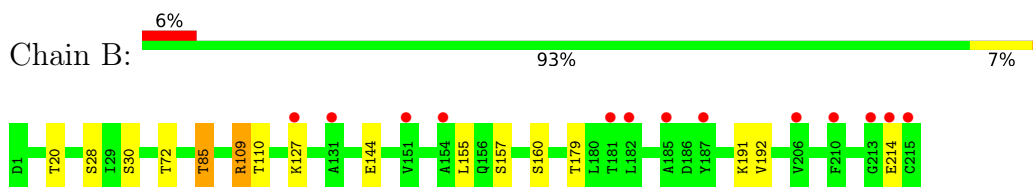
3 Residue-property plots [i](#)

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.

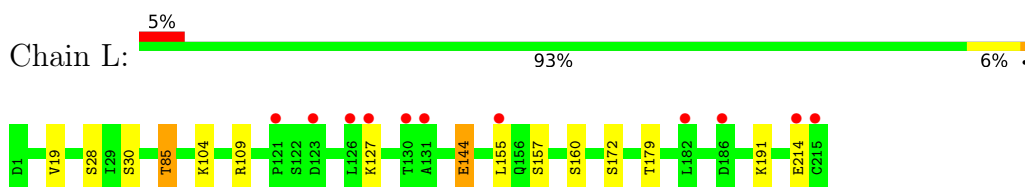
- Molecule 1: anti-CDH6 Fab heavy chain



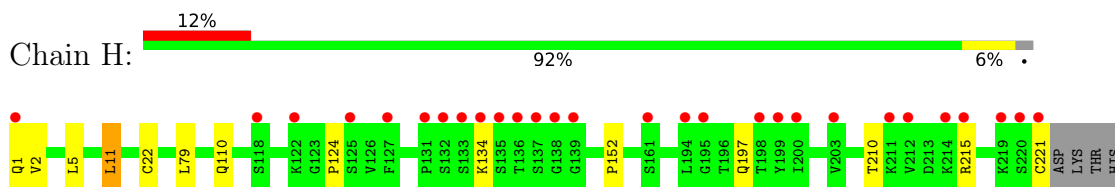
- Molecule 2: anti-CDH6 Fab light chain



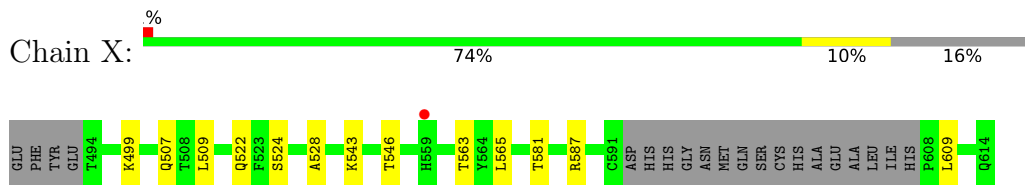
- Molecule 2: anti-CDH6 Fab light chain



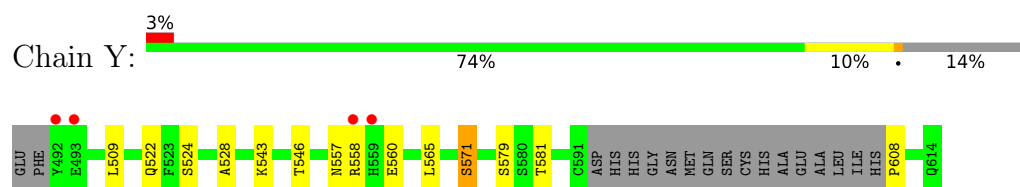
- Molecule 3: anti-CDH6 Fab heavy chain



- 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)	Xtrriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.212 , 0.252 0.218 , 0.259	Depositor DCC
R_{free} test set	2824 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.293	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SLL, A2G

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	0.49	0/1662	0.71	0/2261
2	B	0.53	0/1678	0.75	0/2278
2	L	0.51	0/1678	0.75	0/2278
3	H	0.47	0/1672	0.70	0/2275
4	X	0.50	0/825	0.70	0/1120
4	Y	0.52	0/847	0.72	0/1150
All	All	0.50	0/8362	0.72	0/11362

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	1640	0	1592	6	0
2	B	1643	0	1598	8	0
2	L	1643	0	1598	4	0
3	H	1633	0	1591	4	0
4	X	810	0	776	6	0
4	Y	831	0	791	8	0
5	X	28	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	38	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 2.

All (38) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:Y:579:SER:O	5:Y:2001:A2G:H8B	2.19	0.42
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%)	29	31
2	L	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29	31
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%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	30	SER

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Mol	Chain	Res	Type
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%)	174 (96%)	8 (4%)	28	35
2	B	190/190 (100%)	181 (95%)	9 (5%)	26	33
2	L	190/190 (100%)	181 (95%)	9 (5%)	26	33
3	H	183/187 (98%)	176 (96%)	7 (4%)	33	41
4	X	92/109 (84%)	86 (94%)	6 (6%)	17	19
4	Y	94/109 (86%)	87 (93%)	7 (7%)	13	14
All	All	931/971 (96%)	885 (95%)	46 (5%)	25	31

All (46) 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	215	ARG
1	A	221	CYS
2	B	28	SER
2	B	85	THR
2	B	109	ARG
2	B	127	LYS
2	B	144	GLU
2	B	155	LEU
2	B	157	SER
2	B	191	LYS
2	B	214	GLU

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Mol	Chain	Res	Type
3	H	5	LEU
3	H	11	LEU
3	H	110	GLN
3	H	134	LYS
3	H	197	GLN
3	H	215	ARG
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
2	L	191	LYS
2	L	214	GLU
4	X	499	LYS
4	X	522	GLN
4	X	524	SER
4	X	543	LYS
4	X	565	LEU
4	X	581	THR
4	Y	522	GLN
4	Y	524	SER
4	Y	543	LYS
4	Y	558	ARG
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	211	ASN
3	H	169	HIS
2	L	138	ASN
2	L	148	GLN
2	L	211	ASN
4	X	522	GLN
4	X	542	ASN
4	Y	536	ASN
4	Y	542	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	2.56	4 (28%)	12,17,19	6.13	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	6.08	1.35	1.23
1	A	65	SLL	CX-NZ	4.74	1.44	1.33
1	A	65	SLL	OP1-CP	3.94	1.35	1.22
1	A	65	SLL	OP2-CP	-2.92	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	17.01	154.42	122.84
1	A	65	SLL	CK-CX-NZ	-7.02	104.60	116.42
1	A	65	SLL	CL-CK-CX	6.60	124.12	112.56
1	A	65	SLL	OX-CX-NZ	-5.74	112.19	123.01
1	A	65	SLL	CK-CL-CP	4.16	122.56	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	SLL	OP2-CP-CL	2.67	122.62	114.03
1	A	65	SLL	OX-CX-CK	2.31	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 monosaccharides 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	Y	2001	4	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
5	A2G	X	2002	4	14,14,15	1.26	1 (7%)	17,19,21	3.59	8 (47%)
5	A2G	Y	2002	4	14,14,15	0.76	0	17,19,21	1.10	1 (5%)

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	0.80	0	17,19,21	1.24	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
5	A2G	Y	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	-	5/6/23/26	0/1/1/1
5	A2G	X	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	3.58	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	2002	A2G	C1-O5-C5	7.07	121.77	112.19
5	X	2002	A2G	C3-C4-C5	6.54	121.90	110.24
5	X	2002	A2G	O5-C5-C4	-6.47	95.09	110.83
5	X	2002	A2G	O3-C3-C2	6.03	121.95	109.47
5	X	2002	A2G	C4-C3-C2	-3.97	105.21	111.02
5	Y	2001	A2G	C2-N2-C7	-2.84	118.86	122.90
5	X	2002	A2G	O7-C7-N2	2.76	127.03	121.95
5	Y	2001	A2G	C1-O5-C5	2.71	115.86	112.19
5	X	2002	A2G	C2-N2-C7	2.55	126.53	122.90
5	X	2001	A2G	C1-O5-C5	2.43	115.48	112.19
5	X	2002	A2G	O5-C1-C2	-2.35	107.58	111.29
5	X	2001	A2G	O7-C7-N2	2.20	126.00	121.95
5	Y	2002	A2G	O7-C7-N2	2.16	125.92	121.95

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	2002	A2G	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
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	X	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	Y	2001	A2G	4	0
5	X	2002	A2G	1	0
5	Y	2002	A2G	1	0
5	X	2001	A2G	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, 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%)	0.50	12 (5%) 25 34	16, 36, 79, 114	0
2	B	215/215 (100%)	0.36	13 (6%) 21 30	18, 33, 61, 117	0
2	L	215/215 (100%)	0.36	11 (5%) 28 39	19, 36, 61, 111	0
3	H	221/225 (98%)	0.91	28 (12%) 3 6	18, 46, 81, 118	0
4	X	105/125 (84%)	0.20	1 (0%) 82 88	24, 40, 60, 82	0
4	Y	107/125 (85%)	0.30	4 (3%) 41 52	22, 37, 64, 85	0
All	All	1083/1130 (95%)	0.48	69 (6%) 19 27	16, 38, 72, 118	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	135	SER	16.4
3	H	134	LYS	10.4
3	H	137	SER	10.2
1	A	136	THR	10.1
1	A	135	SER	9.0
3	H	138	GLY	9.0
1	A	137	SER	8.1
3	H	221	CYS	7.9
2	L	215	CYS	6.8
2	B	215	CYS	6.5
1	A	134	LYS	6.4
3	H	132	SER	6.3
4	Y	492	TYR	6.2
3	H	195	GLY	5.9
1	A	220	SER	5.9
1	A	221	CYS	5.7
3	H	136	THR	5.6
1	A	138	GLY	5.3
2	L	127	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	185	ALA	4.6
1	A	132	SER	4.4
3	H	220	SER	4.3
3	H	219	LYS	4.2
1	A	219	LYS	4.2
1	A	133	SER	4.1
2	L	126	LEU	4.1
4	Y	493	GLU	3.9
3	H	198	THR	3.5
4	Y	558	ARG	3.5
3	H	203	VAL	3.4
2	L	155	LEU	3.2
3	H	200	ILE	3.2
2	B	213	GLY	3.2
3	H	194	LEU	3.1
2	L	123	ASP	3.0
2	L	182	LEU	3.0
2	B	181	THR	3.0
3	H	212	VAL	3.0
2	L	130	THR	3.0
3	H	139	GLY	2.8
4	X	559	HIS	2.8
2	B	131	ALA	2.6
3	H	214	LYS	2.5
2	B	127	LYS	2.5
2	B	187	TYR	2.5
2	B	210	PHE	2.5
3	H	199	TYR	2.5
2	L	186	ASP	2.4
3	H	133	SER	2.4
2	L	214	GLU	2.4
4	Y	559	HIS	2.4
3	H	118	SER	2.4
3	H	131	PRO	2.4
2	L	121	PRO	2.4
2	L	131	ALA	2.4
3	H	127	PHE	2.3
2	B	182	LEU	2.3
1	A	126	VAL	2.2
3	H	161	SER	2.2
3	H	215	ARG	2.2
3	H	122	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	H	1	GLN	2.2
3	H	211	LYS	2.1
2	B	214	GLU	2.1
2	B	154	ALA	2.1
2	B	206	VAL	2.1
1	A	215	ARG	2.0
2	B	151	VAL	2.0
3	H	125	SER	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	SLL	A	65	16/17	0.89	0.21	22,42,61,66	0

6.3 Carbohydrates [i](#)

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, 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	0.83	0.20	54,58,72,76	0
5	A2G	X	2002	14/15	0.85	0.22	60,64,77,79	0
5	A2G	Y	2002	14/15	0.85	0.22	59,63,77,77	0
5	A2G	Y	2001	14/15	0.90	0.21	39,49,60,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.