



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2025 – 04:06 PM EDT

PDB ID : 9O6C / pdb_00009o6c
Title : X-ray structure of a bivalent diabody of 8B6, a murine monoclonal antibody specific for the human serotonin transporter
Authors : Coleman, J.A.; Gouaux, E.
Deposited on : 2025-04-12
Resolution : 2.58 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
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) : 2.43.1

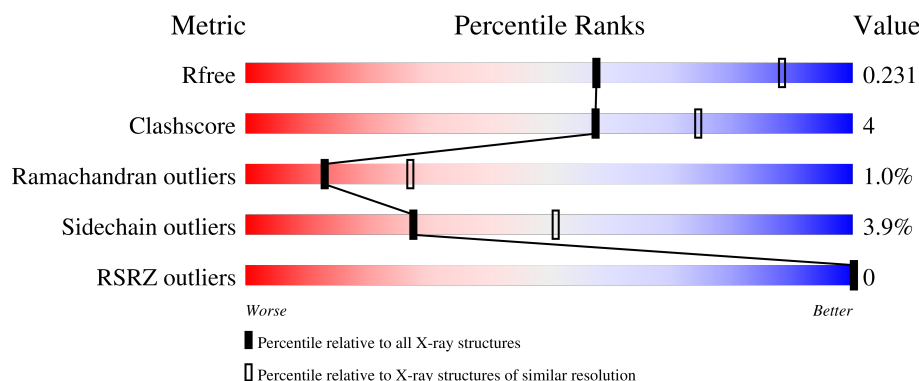
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	234	 45% 6% 50%
1	B	234	 39% 6% 55%
1	C	234	 85% 11% 5% 5%
1	D	234	 83% 14% 3%
1	G	234	 42% 8% 50%

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Mol	Chain	Length	Quality of chain
1	H	234	<div><div></div><div>40%</div><div>5%</div><div>55%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13893 atoms, of which 6754 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 8B6 diabody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	118	Total	C	H	N	O	S	0	0	0
			1821	589	891	153	184	4			
1	B	105	Total	C	H	N	O	S	0	0	0
			1591	511	780	135	161	4			
1	G	118	Total	C	H	N	O	S	0	0	0
			1821	589	891	153	184	4			
1	H	105	Total	C	H	N	O	S	0	0	0
			1591	511	780	135	161	4			
1	C	226	Total	C	H	N	O	S	0	0	0
			3441	1108	1686	292	347	8			
1	D	230	Total	C	H	N	O	S	0	0	0
			3531	1139	1726	306	352	8			

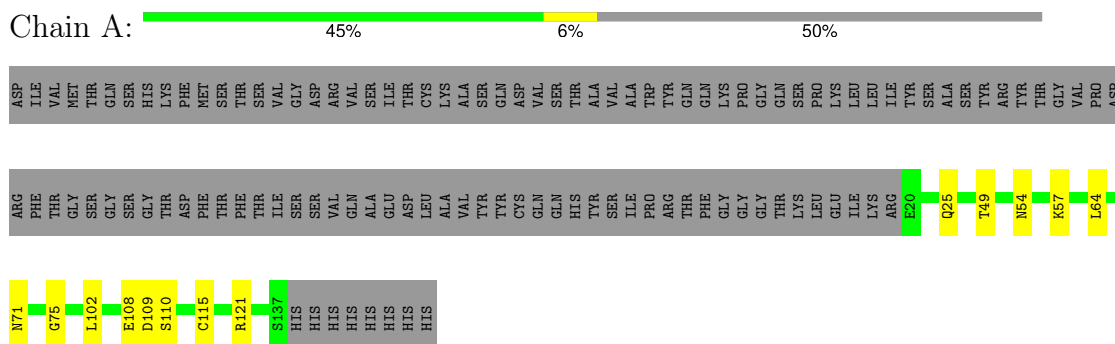
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	14	Total	O	0	0
			14	14		
2	G	20	Total	O	0	0
			20	20		
2	H	11	Total	O	0	0
			11	11		
2	C	23	Total	O	0	0
			23	23		
2	D	13	Total	O	0	0
			13	13		

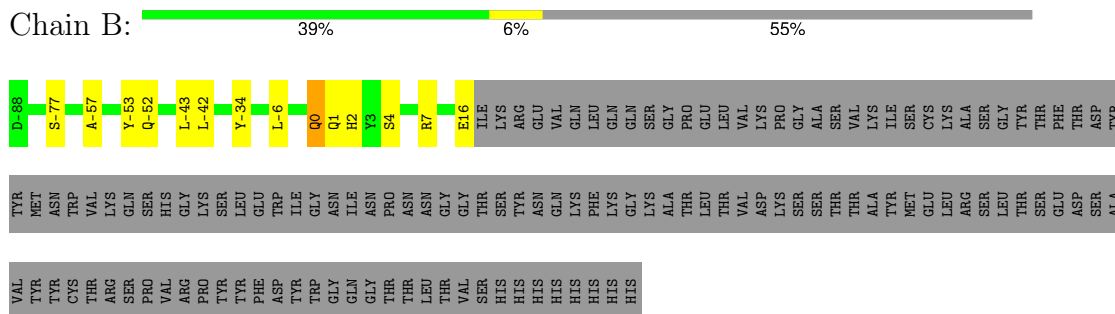
3 Residue-property plots

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.

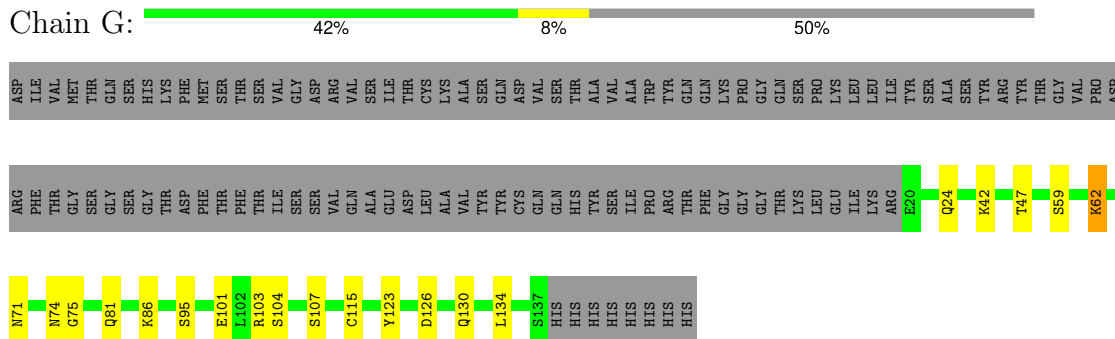
- Molecule 1: 8B6 diabody



- Molecule 1: 8B6 diabody

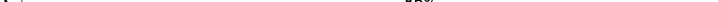


- Molecule 1: 8B6 diabody



- Molecule 1: 8B6 diabody

TYR	ASN	D-88
CYS	TRP	C-66
THR	VAL	K-65
ARG	GLN	A-64
SER	SER	
PRO		W-54
VAL	HIS	
ARG	GLY	R-28
PRO	LYS	F-27
TYR	SER	T-26
TYR	LEU	
PHE	GLU	T-20
ASP	TRP	
ASP	ILE	T-15
TRP	GLY	
THR	ASN	D-7
GLN	ILE	L-6
GLY	ASN	A-5
THR	PRO	
THR	ASN	
LEU	ASN	H2
LEU	GLY	
VAL	GLY	E16
SER	THR	ILE
HIS	SER	LYS
HIS	TYR	ARG
HIS	ASN	GLU
HIS	GLN	VAL
HIS	LYS	GLN
HIS	PHE	LEU
HIS	LYS	GLN
HIS	GLY	SER
	LYS	GLY
	ALA	PRO
	THR	GLU
	LEU	THR
	VAL	LEU
	VAL	VAL
	ASP	LYS
	LYS	PRO
	SER	GLY
	SER	ALA
	SER	ALA
	THR	SER
	THR	VAL
	TYR	ILE
	MET	SER
	LEU	CYS
	GLU	LYS
	LEU	ALA
	SER	SER
	LEU	GLY
	THR	TYR
	SER	THR
	GLU	PHE
	ASP	THR
	SER	ASP
	ALA	TYR
	VAL	THR
	TYR	MET

- Chain C:  85% 11% ...

D-88	G-73	V-70	S-69	T-58	P-49	R-35	T-26	L-6	H2	I17	K18	R19	E20	Q21	G22	L23	V31	C41	T47	F48	T49	N54	M71	G75	K84	G85	K86	L102	R103	S104	R121	S137	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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- Chain D: 83% 14% •

HIS	D-8E
HIS	I-87
HIS	T-84
HIS	Q-83
	V-70
	K-65
	A-57
	Q-47
	Q1
	H2
	T8
	T13
	E16
	I17
	K18
	R19
	E20
	L23
	S36
	I39
	S40
	C41
	T49
	N54
	M55
	V56
	X57
	T77
	S78
	Y79
	L89
	R103
	Y113
	T132
	V136
	S137
	H138
	H139
	H140
	H141

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.47Å 78.47Å 253.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.63 – 2.58 65.63 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.6 (65.63-2.58) 99.6 (65.63-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.58Å)	Xtriage
Refinement program	PHENIX dev_1634	Depositor
R, R_{free}	0.199 , 0.233 0.203 , 0.231	Depositor DCC
R_{free} test set	1475 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.417 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13893	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.30	0/954	0.63	0/1295
1	B	0.31	0/830	0.62	0/1125
1	C	0.29	0/1798	0.61	0/2440
1	D	0.30	0/1853	0.65	0/2515
1	G	0.28	0/954	0.62	0/1295
1	H	0.29	0/830	0.63	0/1125
All	All	0.30	0/7219	0.63	0/9795

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	930	891	891	8	0
1	B	811	780	780	7	0
1	C	1755	1686	1686	15	0
1	D	1805	1726	1726	15	0
1	G	930	891	891	11	0
1	H	811	780	780	7	0
2	A	16	0	0	4	0
2	B	14	0	0	0	0
2	C	23	0	0	5	0
2	D	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	20	0	0	5	0
2	H	11	0	0	2	0
All	All	7139	6754	6754	60	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 4.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-49:PRO:O	1:D:-47:GLN:NE2	2.26	0.69
1:H:-7:ASP:O	2:H:201:HOH:O	2.13	0.67
1:A:121:ARG:NH2	1:C:49:THR:O	2.29	0.66
1:C:-35:ARG:NH1	2:C:205:HOH:O	2.28	0.66
1:H:-65:LYS:NZ	1:H:-64:ALA:O	2.28	0.65
1:A:57:LYS:O	2:A:201:HOH:O	2.15	0.65
1:G:81:GLN:NE2	2:G:208:HOH:O	2.31	0.62
1:C:103:ARG:N	2:C:202:HOH:O	2.31	0.62
1:D:36:SER:OG	1:D:103:ARG:NH1	2.33	0.62
1:G:74:ASN:ND2	2:G:210:HOH:O	2.34	0.61
1:G:74:ASN:ND2	2:G:209:HOH:O	2.32	0.61
1:H:-5:ALA:N	2:H:201:HOH:O	2.29	0.59
1:A:115:CYS:N	2:A:202:HOH:O	2.35	0.58
1:G:130:GLN:O	2:G:201:HOH:O	2.18	0.57
1:G:86:LYS:NZ	1:G:104:SER:O	2.29	0.55
1:C:71:ASN:O	1:C:75:GLY:N	2.39	0.55
1:G:107:SER:N	2:G:211:HOH:O	2.39	0.55
1:D:-84:THR:N	1:D:-65:LYS:O	2.39	0.54
1:C:-73:GLY:O	2:C:201:HOH:O	2.18	0.54
1:A:71:ASN:O	1:A:75:GLY:N	2.39	0.52
1:B:2:HIS:O	1:B:2:HIS:ND1	2.43	0.51
1:G:101:GLU:OE2	1:G:103:ARG:NH1	2.43	0.51
1:A:49:THR:O	1:C:121:ARG:NH2	2.43	0.51
1:G:81:GLN:OE1	1:G:81:GLN:N	2.41	0.49
1:D:-83:GLN:NE2	1:D:13:THR:OG1	2.44	0.48
1:H:-28:ARG:NH2	1:H:-7:ASP:OD1	2.44	0.46
1:C:86:LYS:NZ	1:C:104:SER:O	2.48	0.46
1:C:-59:SER:OG	1:C:-58:THR:N	2.48	0.46
1:B:-53:TYR:HE1	1:B:0:GLN:HG2	1.81	0.46
1:C:2:HIS:ND1	1:C:2:HIS:O	2.49	0.46
1:D:79:TYR:OH	1:D:89:LEU:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-57:ALA:HA	1:D:2:HIS:CE1	2.51	0.45
1:B:4:SER:O	1:B:7:ARG:NH1	2.49	0.45
1:A:25:GLN:OE1	2:A:202:HOH:O	2.21	0.45
1:A:108:GLU:OE1	1:A:109:ASP:N	2.49	0.45
1:A:64:LEU:HA	2:A:201:HOH:O	2.17	0.45
1:D:13:THR:O	2:D:201:HOH:O	2.20	0.45
1:G:71:ASN:O	1:G:75:GLY:N	2.46	0.44
1:C:84:LYS:NZ	2:C:211:HOH:O	2.50	0.44
1:D:55:TRP:CD1	1:D:89:LEU:HD21	2.52	0.44
1:D:16:GLU:CG	1:D:17:ILE:H	2.31	0.44
1:G:59:SER:HB2	1:G:62:LYS:HD3	2.00	0.43
1:C:-6:LEU:HD11	1:C:17:ILE:HG23	1.99	0.43
1:B:-52:GLN:HB2	1:B:-42:LEU:HD11	2.00	0.43
1:C:86:LYS:O	2:C:202:HOH:O	2.22	0.43
1:D:23:LEU:HD21	1:D:41:CYS:SG	2.60	0.42
1:D:57:LYS:NZ	1:D:113:TYR:OH	2.45	0.42
1:B:-43:LEU:HD22	1:B:-34:TYR:HB2	2.02	0.42
1:H:-66:CYS:HB2	1:H:-54:TRP:CH2	2.55	0.42
1:G:42:LYS:NZ	1:G:95:SER:O	2.46	0.42
1:D:39:ILE:HD11	1:D:132:THR:HG21	2.02	0.42
1:D:16:GLU:HG2	1:D:17:ILE:H	1.85	0.42
1:H:-26:THR:HG23	1:H:-15:THR:HB	2.02	0.41
1:C:23:LEU:HD21	1:C:41:CYS:SG	2.60	0.41
1:D:-87:ILE:O	1:D:8:THR:OG1	2.37	0.41
1:C:31:VAL:O	1:C:137:SER:N	2.44	0.41
1:D:77:THR:HG21	1:D:79:TYR:CZ	2.56	0.41
1:B:-77:SER:HA	1:B:16:GLU:HB2	2.04	0.40
1:B:-57:ALA:HA	1:B:2:HIS:CE1	2.57	0.40
1:H:2:HIS:ND1	1:H:2:HIS:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	116/234 (50%)	111 (96%)	4 (3%)	1 (1%)	14	30
1	B	103/234 (44%)	95 (92%)	8 (8%)	0	100	100
1	C	224/234 (96%)	208 (93%)	13 (6%)	3 (1%)	10	20
1	D	228/234 (97%)	203 (89%)	20 (9%)	5 (2%)	5	10
1	G	116/234 (50%)	112 (97%)	4 (3%)	0	100	100
1	H	103/234 (44%)	93 (90%)	10 (10%)	0	100	100
All	All	890/1404 (63%)	822 (92%)	59 (7%)	9 (1%)	13	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	LYS
1	D	140	HIS
1	D	138	HIS
1	C	18	LYS
1	D	20	GLU
1	A	110	SER
1	C	21	VAL
1	C	17	ILE
1	D	17	ILE

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	103/204 (50%)	101 (98%)	2 (2%)	52	74
1	B	90/204 (44%)	87 (97%)	3 (3%)	33	57
1	C	193/204 (95%)	186 (96%)	7 (4%)	30	54
1	D	199/204 (98%)	189 (95%)	10 (5%)	20	41
1	G	103/204 (50%)	96 (93%)	7 (7%)	13	27
1	H	90/204 (44%)	89 (99%)	1 (1%)	70	86
All	All	778/1224 (64%)	748 (96%)	30 (4%)	27	51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	102	LEU
1	B	-6	LEU
1	B	0	GLN
1	B	1	GLN
1	G	24	GLN
1	G	47	THR
1	G	62	LYS
1	G	115	CYS
1	G	123	TYR
1	G	126	ASP
1	G	134	LEU
1	H	-20	THR
1	C	-70	VAL
1	C	-26	THR
1	C	18	LYS
1	C	20	GLU
1	C	47	THR
1	C	54	ASN
1	C	102	LEU
1	D	-70	VAL
1	D	1	GLN
1	D	17	ILE
1	D	19	ARG
1	D	49	THR
1	D	54	ASN
1	D	77	THR
1	D	136	VAL
1	D	137	SER
1	D	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-47	GLN
1	H	-47	GLN
1	C	22	GLN
1	C	58	GLN
1	D	-51	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	118/234 (50%)	-1.29	0 100 100	69, 96, 135, 195	0
1	B	105/234 (44%)	-1.29	0 100 100	45, 77, 112, 137	0
1	C	226/234 (96%)	-1.22	0 100 100	64, 101, 162, 312	0
1	D	230/234 (98%)	-1.13	0 100 100	60, 120, 208, 322	0
1	G	118/234 (50%)	-1.05	0 100 100	86, 137, 203, 315	0
1	H	105/234 (44%)	-1.13	0 100 100	78, 123, 168, 261	0
All	All	902/1404 (64%)	-1.18	0 100 100	45, 110, 183, 322	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.