



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:31 AM UTC

PDB ID : 6DG2 / pdb_00006dg2
Title : Antigen Binding Fragment of the Pan-ebolavirus Monoclonal Antibody 6D6
Authors : Milligan, J.C.; Sapphire, E.O.
Deposited on : 2018-05-16
Resolution : 1.96 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
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

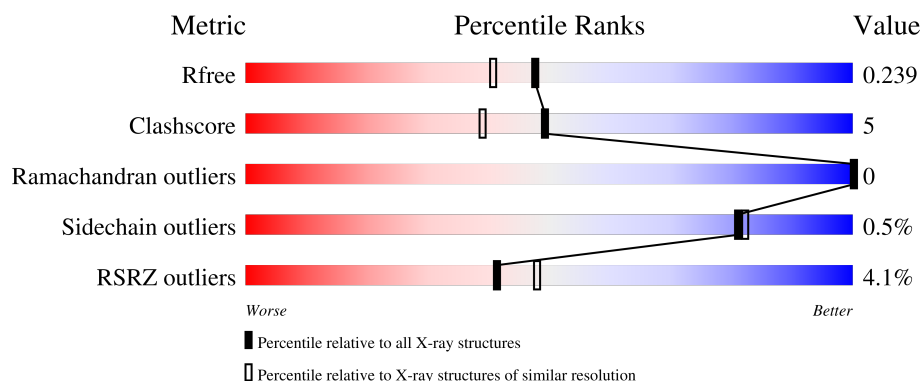
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	230	3% 83% 10% 6%
1	C	230	4% 82% 9% 8%
2	B	215	2% 91% 7% .
2	D	215	6% 80% 17% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6846 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 6D6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1632	1035	270	322	5			
1	C	211	Total	C	N	O	S	0	0	0
			1601	1017	264	315	5			

- Molecule 2 is a protein called 6D6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1640	1031	277	326	6			
2	D	211	Total	C	N	O	S	0	0	0
			1636	1029	276	325	6			

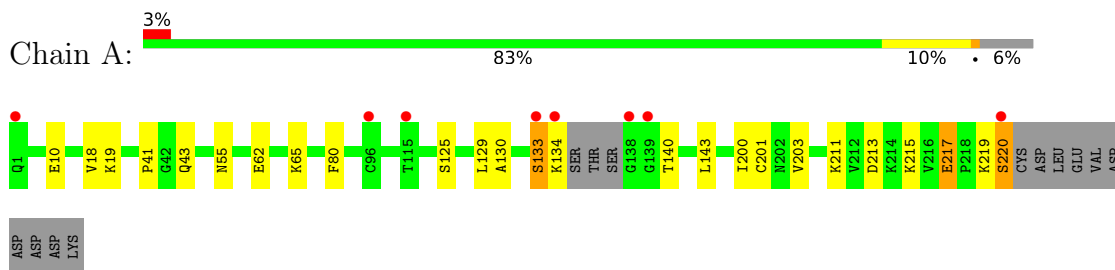
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	B	86	Total	O	0	0
			86	86		
3	C	92	Total	O	0	0
			92	92		
3	D	55	Total	O	0	0
			55	55		

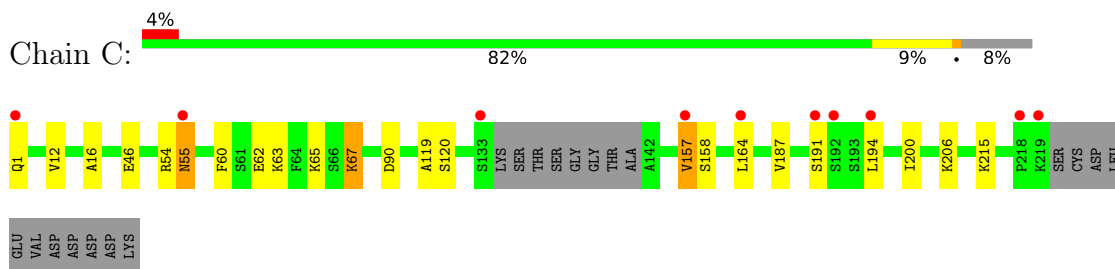
3 Residue-property plots [i](#)

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.

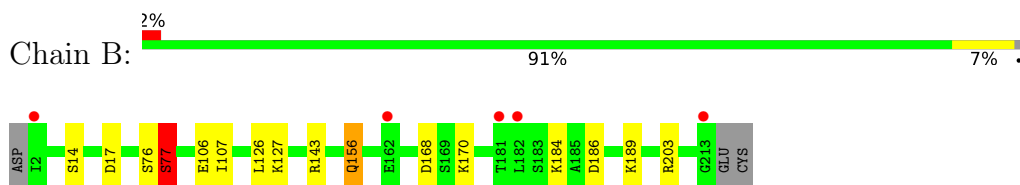
- Molecule 1: 6D6 Fab heavy chain



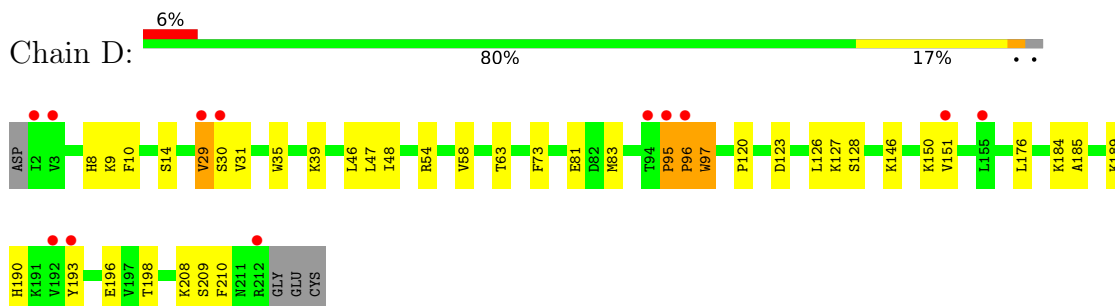
- Molecule 1: 6D6 Fab heavy chain



- Molecule 2: 6D6 Fab light chain



- Molecule 2: 6D6 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.23Å 72.04Å 107.15Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	68.08 – 1.96 68.08 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.5 (68.08-1.96) 93.5 (68.08-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.191 , 0.235 0.199 , 0.239	Depositor DCC
R_{free} test set	1978 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6846	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

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	0.78	3/1675 (0.2%)	0.75	6/2283 (0.3%)
1	C	0.82	1/1644 (0.1%)	0.87	7/2242 (0.3%)
2	B	0.61	1/1677 (0.1%)	0.79	6/2277 (0.3%)
2	D	0.50	1/1673 (0.1%)	0.82	12/2272 (0.5%)
All	All	0.69	6/6669 (0.1%)	0.81	31/9074 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	ALA	C-N	-25.89	0.93	1.33
2	B	77	SER	C-N	-19.28	1.05	1.33
2	D	208	LYS	C-N	14.88	1.51	1.33
1	A	201	CYS	C-N	-14.86	1.12	1.33
1	A	200	ILE	C-N	10.52	1.48	1.33
1	A	130	ALA	C-O	-5.36	1.17	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	SER	O-C-N	-16.82	102.75	123.27
1	C	157	VAL	N-CA-C	15.02	140.57	109.34
2	D	30	SER	N-CA-C	13.21	127.14	111.02
1	C	157	VAL	CB-CA-C	-12.97	90.01	111.29
1	A	133	SER	N-CA-C	12.78	124.95	111.14
1	C	158	SER	N-CA-C	12.08	125.91	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	SER	CA-C-N	-11.67	103.83	122.73
2	B	76	SER	C-N-CA	-11.67	103.83	122.73
2	D	8	HIS	N-CA-C	11.41	124.26	110.91
1	C	194	LEU	N-CA-C	8.79	122.58	111.24
1	C	120	SER	O-C-N	-7.57	114.03	123.27
2	D	96	PRO	N-CA-C	-7.38	97.26	112.47
1	A	133	SER	CB-CA-C	-7.34	99.30	110.90
1	A	130	ALA	N-CA-C	7.11	118.75	109.93
2	D	29	VAL	N-CA-C	-6.99	96.83	107.73
2	D	30	SER	CB-CA-C	-6.74	100.21	110.92
2	B	77	SER	CA-C-N	6.70	130.91	121.66
2	B	77	SER	C-N-CA	6.70	130.91	121.66
2	D	97	TRP	N-CA-C	-6.61	100.49	109.54
2	B	143	ARG	N-CA-C	6.51	119.20	111.33
2	D	31	VAL	N-CA-CB	6.25	121.55	111.23
1	C	67	LYS	N-CA-C	6.04	120.78	113.41
2	D	8	HIS	CB-CA-C	-5.84	102.05	112.27
2	D	95	PRO	N-CA-C	5.70	117.65	110.70
1	C	158	SER	N-CA-CB	-5.56	102.73	110.29
2	D	209	SER	O-C-N	5.54	129.68	123.48
1	A	129	LEU	N-CA-C	-5.32	97.15	107.62
2	D	209	SER	CA-C-N	-5.26	112.65	121.75
2	D	209	SER	C-N-CA	-5.26	112.65	121.75
1	A	217	GLU	CA-C-N	-5.17	114.63	119.85
1	A	217	GLU	C-N-CA	-5.17	114.63	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	SER	Mainchain

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	1632	0	1584	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1601	0	1555	14	0
2	B	1640	0	1594	12	0
2	D	1636	0	1592	26	0
3	A	104	0	0	2	0
3	B	86	0	0	3	0
3	C	92	0	0	3	0
3	D	55	0	0	4	0
All	All	6846	0	6325	69	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 5.

All (69) 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:157:VAL:O	1:C:157:VAL:CG1	1.81	1.23
1:C:1:GLN:N	3:C:301:HOH:O	1.65	1.16
2:D:146:LYS:HB3	2:D:198:THR:HG22	1.41	1.01
1:C:157:VAL:O	1:C:157:VAL:HG12	1.03	0.90
2:D:128:SER:OG	3:D:301:HOH:O	1.92	0.87
1:A:125:SER:OG	3:A:301:HOH:O	2.00	0.78
1:A:219:LYS:HG2	1:A:220:SER:N	2.01	0.73
1:A:219:LYS:HG2	1:A:220:SER:H	1.58	0.69
1:A:41:PRO:O	1:A:43:GLN:NE2	2.25	0.67
2:B:106:GLU:OE1	3:B:302:HOH:O	2.15	0.65
1:A:133:SER:OG	1:A:134:LYS:N	2.29	0.65
1:C:54:ARG:NH1	3:C:302:HOH:O	2.31	0.63
1:A:211:LYS:NZ	1:A:213:ASP:OD1	2.32	0.63
2:D:123:ASP:HA	2:D:126:LEU:HD12	1.81	0.62
2:B:156:GLN:HE21	2:B:156:GLN:HA	1.64	0.62
2:B:168:ASP:OD1	2:B:170:LYS:HG2	2.02	0.60
2:D:95:PRO:O	2:D:96:PRO:C	2.41	0.60
1:C:60:PHE:HB2	1:C:65:LYS:HG2	1.84	0.59
1:C:67:LYS:HE2	1:C:90:ASP:OD2	2.02	0.59
2:B:203:ARG:CD	3:B:301:HOH:O	2.51	0.58
2:D:29:VAL:O	2:D:29:VAL:HG23	2.03	0.58
1:A:140:THR:HG23	1:A:140:THR:O	2.04	0.57
2:D:127:LYS:HA	2:D:184:LYS:NZ	2.21	0.56
2:B:186:ASP:OD1	2:B:189:LYS:NZ	2.38	0.53
2:D:47:LEU:O	2:D:48:ILE:HG13	2.08	0.53
2:B:203:ARG:HD3	3:B:301:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ARG:HG2	2:D:58:VAL:HB	1.93	0.51
2:B:106:GLU:HG2	2:B:107:ILE:N	2.24	0.51
1:C:62:GLU:OE1	1:C:65:LYS:HE3	2.11	0.51
2:D:127:LYS:HA	2:D:184:LYS:HZ3	1.76	0.51
2:D:127:LYS:HD2	2:D:127:LYS:C	2.35	0.51
1:C:206:LYS:HG3	3:C:387:HOH:O	2.11	0.51
1:A:62:GLU:OE1	1:A:65:LYS:NZ	2.45	0.50
2:D:83:MET:N	2:D:83:MET:SD	2.84	0.49
2:D:150:LYS:NZ	2:D:196:GLU:OE2	2.44	0.49
2:D:9:LYS:HD2	3:D:316:HOH:O	2.14	0.48
1:C:46:GLU:OE2	1:C:63:LYS:HD3	2.12	0.48
2:D:95:PRO:O	2:D:97:TRP:N	2.46	0.48
1:A:203:VAL:O	1:A:211:LYS:HD2	2.13	0.48
1:C:164:LEU:HD21	1:C:187:VAL:HG21	1.95	0.48
1:A:219:LYS:CG	1:A:220:SER:N	2.76	0.48
2:D:120:PRO:HB3	2:D:210:PHE:CE1	2.49	0.47
1:A:19:LYS:HE3	1:A:80:PHE:CD2	2.50	0.46
2:D:54:ARG:HH21	2:D:63:THR:HG22	1.79	0.46
2:B:127:LYS:HB3	2:B:127:LYS:HE2	1.72	0.46
2:B:126:LEU:O	2:B:184:LYS:HE2	2.15	0.46
1:A:143:LEU:C	1:A:143:LEU:HD12	2.41	0.45
1:A:215:LYS:HG2	1:A:217:GLU:OE2	2.16	0.45
2:B:17:ASP:O	2:B:77:SER:HA	2.17	0.45
1:A:55:ASN:ND2	3:A:307:HOH:O	2.50	0.44
2:D:151:VAL:HG12	2:D:193:TYR:CD1	2.51	0.44
2:B:126:LEU:O	2:B:184:LYS:HD3	2.18	0.44
2:D:10:PHE:HB3	3:D:328:HOH:O	2.17	0.43
2:D:35:TRP:CE2	2:D:73:PHE:HB2	2.54	0.43
2:D:189:LYS:HB2	2:D:190:HIS:CE1	2.54	0.42
1:C:200:ILE:HG12	1:C:215:LYS:HB2	2.02	0.42
2:D:185:ALA:O	2:D:189:LYS:HE2	2.20	0.42
2:D:46:LEU:O	2:D:47:LEU:HD23	2.20	0.41
2:B:14:SER:HB2	2:B:17:ASP:OD2	2.20	0.41
1:C:12:VAL:HG13	1:C:16:ALA:HB3	2.00	0.41
1:A:219:LYS:CG	1:A:220:SER:H	2.30	0.41
1:C:62:GLU:HA	1:C:65:LYS:HE2	2.02	0.41
2:D:39:LYS:NZ	2:D:81:GLU:HG2	2.36	0.41
2:D:176:LEU:HD23	2:D:176:LEU:C	2.46	0.41
2:D:95:PRO:O	2:D:97:TRP:CD1	2.74	0.41
1:A:215:LYS:HG2	1:A:217:GLU:HG3	2.02	0.40
1:A:10:GLU:HG2	1:A:18:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ASN:HD22	1:C:55:ASN:HA	1.66	0.40
2:D:14:SER:OG	3:D:302:HOH:O	2.22	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	213/230 (93%)	207 (97%)	6 (3%)	0	100	100
1	C	207/230 (90%)	200 (97%)	7 (3%)	0	100	100
2	B	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
2	D	209/215 (97%)	191 (91%)	18 (9%)	0	100	100
All	All	839/890 (94%)	799 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	183/198 (92%)	182 (100%)	1 (0%)	81	82
1	C	181/198 (91%)	179 (99%)	2 (1%)	65	64
2	B	186/189 (98%)	185 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	186/189 (98%)	186 (100%)	0	100	100
All	All	736/774 (95%)	732 (100%)	4 (0%)	81	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	SER
2	B	156	GLN
1	C	55	ASN
1	C	191	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	197	GLN
2	B	38	GLN
2	B	156	GLN
1	C	39	GLN
1	C	43	GLN
1	C	197	GLN
2	D	37	GLN
2	D	38	GLN
2	D	42	GLN
2	D	148	GLN
2	D	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
2	B	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	201:CYS	C	202:ASN	N	1.12
1	B	77:SER	C	78:VAL	N	1.05
1	C	119:ALA	C	120:SER	N	0.93

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	217/230 (94%)	0.24	8 (3%) 45 52	29, 42, 74, 116	0
1	C	211/230 (91%)	0.34	10 (4%) 36 42	28, 45, 92, 118	0
2	B	212/215 (98%)	0.29	5 (2%) 59 66	31, 50, 79, 88	0
2	D	211/215 (98%)	0.55	12 (5%) 29 34	32, 56, 94, 113	0
All	All	851/890 (95%)	0.35	35 (4%) 41 48	28, 48, 83, 118	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	SER	5.5
2	D	2	ILE	5.2
2	D	96	PRO	4.9
2	B	213	GLY	4.8
1	A	138	GLY	4.3
2	D	95	PRO	4.2
2	D	29	VAL	3.9
1	C	133	SER	3.7
2	D	30	SER	3.3
1	C	218	PRO	3.3
1	A	134	LYS	3.3
1	A	96	CYS	3.1
1	A	133	SER	3.1
2	D	155	LEU	2.8
1	A	1	GLN	2.8
2	D	94	THR	2.7
1	C	194	LEU	2.7
1	A	139	GLY	2.6
1	C	219	LYS	2.6
1	C	157	VAL	2.6
1	C	55	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	212	ARG	2.5
1	C	1	GLN	2.5
2	D	3	VAL	2.5
1	A	115	THR	2.5
1	C	164	LEU	2.3
2	D	151	VAL	2.3
2	B	2	ILE	2.3
2	D	193	TYR	2.2
2	B	182	LEU	2.2
2	D	192	VAL	2.2
2	B	162	GLU	2.1
1	C	191	SER	2.1
1	C	192	SER	2.1
2	B	181	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.