Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 05:59 AM EDT

PDB ID	:	6BGT
Title	:	Structure of Trastuzumab Fab mutant in complex with Her2 extracellular domain
Authors	:	Christie, M.; Christ, D.
Deposited on	:	2017-10-29
Resolution	:	2.70 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:

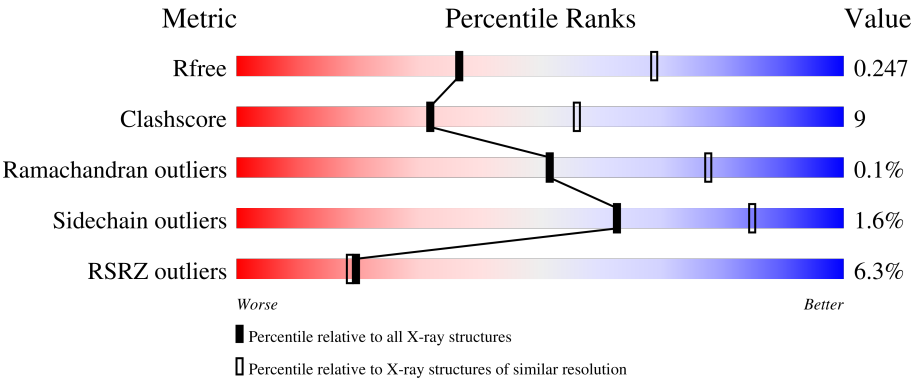
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	C	658	% 75% 14% 10%
2	A	214	13% 77% 21%
3	B	231	13% 70% 20% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7806 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	589	Total	C	N	O	S	0	0	0
			4547	2829	813	852	53			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	631	HIS	-	expression tag	UNP P04626
C	632	HIS	-	expression tag	UNP P04626
C	633	HIS	-	expression tag	UNP P04626
C	634	HIS	-	expression tag	UNP P04626
C	635	HIS	-	expression tag	UNP P04626
C	636	HIS	-	expression tag	UNP P04626

- Molecule 2 is a protein called Herceptin light chain mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	211	Total	C	N	O	S	0	0	0
			1632	1023	274	330	5			

- Molecule 3 is a protein called Herceptin heavy chain Fab fragment mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	210	Total	C	N	O	S	0	0	0
			1584	1004	266	308	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	224	GLY	-	expression tag	UNP P0DOX5
B	225	SER	-	expression tag	UNP P0DOX5
B	226	HIS	-	expression tag	UNP P0DOX5
B	227	HIS	-	expression tag	UNP P0DOX5

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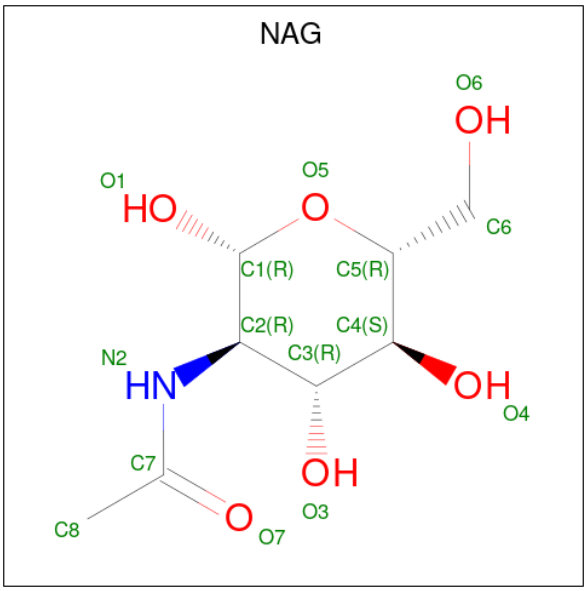
Chain	Residue	Modelled	Actual	Comment	Reference
B	228	HIS	-	expression tag	UNP P0DOX5
B	229	HIS	-	expression tag	UNP P0DOX5
B	230	HIS	-	expression tag	UNP P0DOX5
B	231	HIS	-	expression tag	UNP P0DOX5

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

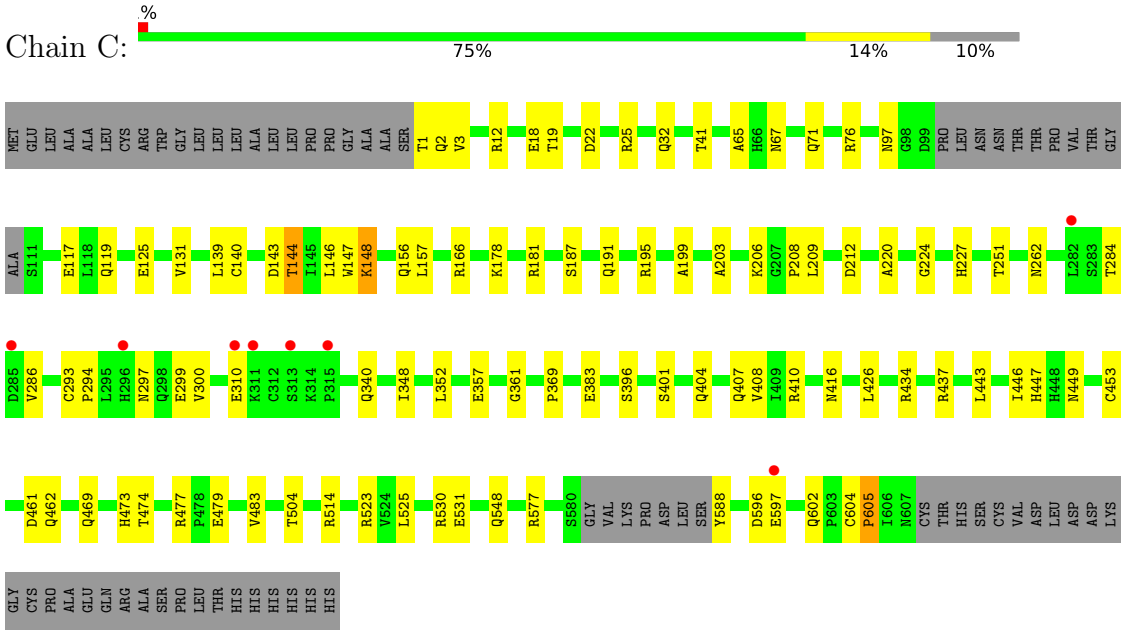
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	28	Total O 28 28	0	0
5	A	1	Total O 1 1	0	0

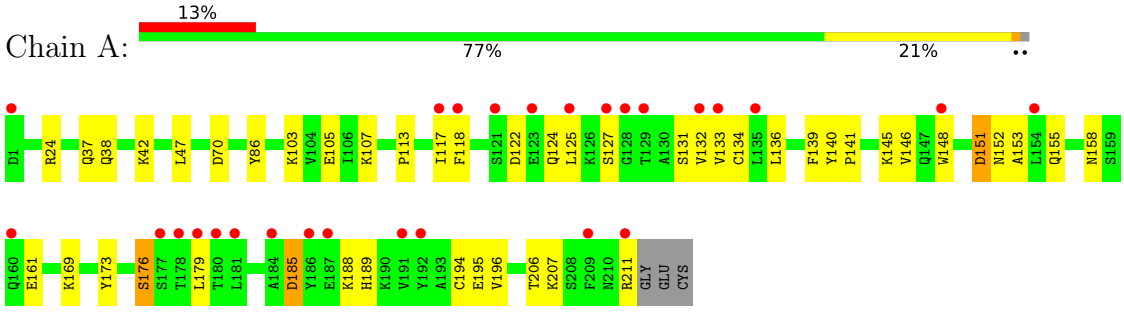
3 Residue-property plots (i)

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.

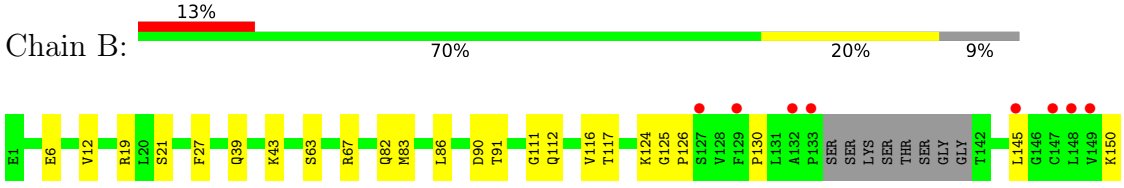
• Molecule 1: Receptor tyrosine-protein kinase erbB-2

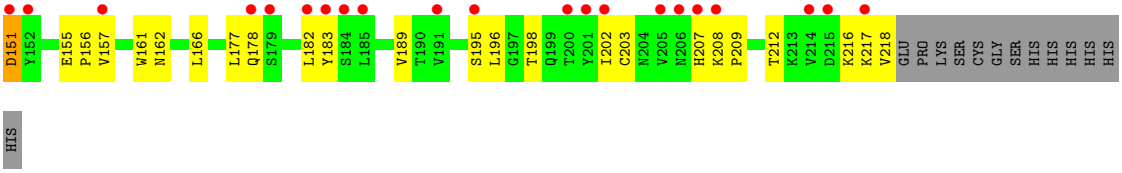


• Molecule 2: Herceptin light chain mutant



• Molecule 3: Herceptin heavy chain Fab fragment mutant




D151
V152
E155
P156
V157
W161
N162
L166
L177
Q178
S179
L182
Y183
S184
L185
V189
T190
V191
S195
L196
G197
T198
Q199
T200
Y201
I202
C203
N204
V205
N206
H207
K208
P209
T212
K213
V214
D215
K216
K217
V218
GLU
PRO
LYS
SER
CYS
GLY
SER
HIS
HIS
HIS
HIS
HIS

HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.86Å 114.46Å 204.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 2.70 53.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.93-2.70) 99.0 (53.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.247 0.205 , 0.247	Depositor DCC
R_{free} test set	2008 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7806	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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	C	0.29	0/4656	0.53	0/6335
2	A	0.35	0/1669	0.58	1/2270 (0.0%)
3	B	0.30	0/1624	0.54	0/2216
All	All	0.31	0/7949	0.54	1/10821 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	151	ASP	CB-CG-OD1	5.29	123.06	118.30

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	C	4547	0	4345	64	0
2	A	1632	0	1585	41	0
3	B	1584	0	1537	34	0
4	C	14	0	13	0	0
5	A	1	0	0	0	0
5	C	28	0	0	6	0
All	All	7806	0	7480	136	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 9.

All (136) 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:148:LYS:O	1:C:156:GLN:NE2	2.10	0.84
1:C:156:GLN:OE1	1:C:195:ARG:NH2	2.11	0.83
1:C:588:TYR:OH	3:B:27:PHE:HB2	1.78	0.82
2:A:195:GLU:OE1	2:A:207:LYS:N	2.16	0.79
2:A:37:GLN:HB2	2:A:47:LEU:HD11	1.65	0.79
2:A:195:GLU:OE1	2:A:206:THR:HA	1.83	0.79
1:C:18:GLU:OE2	5:C:802:HOH:O	2.01	0.78
1:C:25:ARG:NH1	5:C:805:HOH:O	2.18	0.76
2:A:38:GLN:HE22	3:B:39:GLN:HE22	1.32	0.76
1:C:187:SER:OG	5:C:803:HOH:O	2.03	0.76
3:B:91:THR:HG23	3:B:117:THR:HA	1.67	0.76
2:A:148:TRP:CZ3	2:A:194:CYS:HB2	2.23	0.74
1:C:148:LYS:HB3	1:C:156:GLN:HE21	1.55	0.71
3:B:166:LEU:HD21	3:B:189:VAL:HG21	1.73	0.71
1:C:284:THR:HG22	1:C:286:VAL:H	1.54	0.70
1:C:401:SER:O	1:C:404:GLN:HG3	1.91	0.70
1:C:596:ASP:OD2	1:C:597:GLU:N	2.25	0.70
2:A:105:GLU:OE1	2:A:173:TYR:OH	2.08	0.70
1:C:2:GLN:HG3	1:C:3:VAL:HG23	1.74	0.69
1:C:117:GLU:OE2	5:C:804:HOH:O	2.08	0.69
2:A:24:ARG:NH2	2:A:70:ASP:OD1	2.25	0.69
2:A:42:LYS:HD3	3:B:112:GLN:HE22	1.57	0.68
2:A:153:ALA:O	2:A:155:GLN:NE2	2.24	0.68
1:C:514:ARG:NH1	1:C:531:GLU:OE1	2.27	0.67
3:B:126:PRO:HD2	3:B:212:THR:HG21	1.76	0.67
3:B:130:PRO:HB3	3:B:218:VAL:HG12	1.76	0.67
1:C:446:ILE:O	1:C:473:HIS:HA	1.96	0.65
2:A:195:GLU:CD	2:A:206:THR:HA	2.17	0.65
1:C:146:LEU:H	1:C:191:GLN:HE22	1.44	0.65
2:A:132:VAL:HG12	2:A:179:LEU:HB3	1.81	0.63
2:A:136:LEU:HD11	2:A:196:VAL:HG21	1.80	0.63
3:B:83:MET:HE1	3:B:116:VAL:HG21	1.82	0.62
1:C:148:LYS:H	1:C:148:LYS:HD2	1.66	0.61
3:B:67:ARG:NH2	3:B:90:ASP:OD2	2.32	0.61
1:C:144:THR:HG23	1:C:181:ARG:HA	1.82	0.61
1:C:461:ASP:OD2	1:C:462:GLN:NE2	2.34	0.60
1:C:12:ARG:NH1	1:C:416:ASN:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:O	1:C:166:ARG:NH1	2.36	0.58
1:C:426:LEU:H	1:C:449:ASN:HD22	1.50	0.58
1:C:426:LEU:H	1:C:449:ASN:ND2	2.02	0.58
1:C:125:GLU:OE2	1:C:220:ALA:N	2.32	0.57
2:A:185:ASP:HA	2:A:188:LYS:HD2	1.87	0.57
2:A:132:VAL:CG1	2:A:179:LEU:HB3	2.35	0.56
2:A:146:VAL:HG22	2:A:161:GLU:OE1	2.06	0.55
3:B:6:GLU:OE2	3:B:111:GLY:HA3	2.06	0.55
1:C:361:GLY:H	1:C:369:PRO:HG3	1.72	0.54
1:C:2:GLN:HB2	1:C:32:GLN:HE21	1.73	0.53
2:A:195:GLU:HG3	2:A:206:THR:HG22	1.90	0.53
2:A:117:ILE:HG22	2:A:207:LYS:HG2	1.91	0.53
2:A:151:ASP:OD2	2:A:189:HIS:CD2	2.61	0.53
3:B:124:LYS:NZ	3:B:125:GLY:O	2.32	0.52
1:C:144:THR:CG2	1:C:181:ARG:HA	2.40	0.52
2:A:195:GLU:OE1	2:A:195:GLU:HA	2.09	0.52
1:C:140:CYS:HA	1:C:166:ARG:NH1	2.25	0.52
3:B:195:SER:O	3:B:198:THR:HG22	2.10	0.52
1:C:523:ARG:HB2	1:C:531:GLU:HG3	1.91	0.51
3:B:145:LEU:HD13	3:B:218:VAL:HG21	1.91	0.51
1:C:357:GLU:OE1	5:C:806:HOH:O	2.19	0.51
2:A:113:PRO:HB3	2:A:139:PHE:HB3	1.92	0.51
3:B:177:LEU:HB2	3:B:183:TYR:CE1	2.46	0.50
2:A:140:TYR:CG	2:A:141:PRO:HA	2.46	0.50
1:C:76:ARG:NH1	5:C:809:HOH:O	2.45	0.50
1:C:348:ILE:HD13	1:C:352:LEU:HD21	1.92	0.50
1:C:479:GLU:O	1:C:483:VAL:HG23	2.11	0.50
3:B:207:HIS:CD2	3:B:209:PRO:HG2	2.46	0.50
1:C:22:ASP:OD2	1:C:22:ASP:N	2.45	0.50
3:B:196:LEU:H	3:B:196:LEU:HD23	1.77	0.50
1:C:71:GLN:HE22	1:C:119:GLN:HB2	1.76	0.50
3:B:162:ASN:ND2	3:B:202:ILE:HG22	2.26	0.49
1:C:199:ALA:HB2	1:C:208:PRO:O	2.13	0.49
1:C:530:ARG:NH1	1:C:548:GLN:O	2.45	0.49
1:C:251:THR:HG23	1:C:262:ASN:HB2	1.94	0.49
3:B:12:VAL:HG11	3:B:86:LEU:HD13	1.94	0.49
2:A:37:GLN:HG3	2:A:86:TYR:CE1	2.48	0.49
2:A:195:GLU:CD	2:A:207:LYS:H	2.15	0.49
2:A:195:GLU:OE1	2:A:206:THR:CA	2.58	0.48
1:C:67:ASN:H	1:C:97:ASN:HD22	1.59	0.48
1:C:407:GLN:HG2	1:C:437:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LEU:N	1:C:191:GLN:HE22	2.10	0.48
2:A:148:TRP:CH2	2:A:194:CYS:HB2	2.48	0.48
1:C:443:LEU:HD23	1:C:469:GLN:HA	1.94	0.47
1:C:453:CYS:SG	1:C:477:ARG:HD3	2.54	0.47
2:A:124:GLN:O	2:A:127:SER:OG	2.26	0.47
3:B:150:LYS:HG3	3:B:151:ASP:OD1	2.15	0.47
3:B:161:TRP:HB3	3:B:166:LEU:HD23	1.97	0.47
3:B:178:GLN:HG2	3:B:182:LEU:O	2.15	0.47
3:B:151:ASP:HB3	3:B:182:LEU:HD12	1.97	0.47
1:C:195:ARG:HG3	1:C:203:ALA:O	2.14	0.46
2:A:194:CYS:O	2:A:195:GLU:OE1	2.33	0.46
1:C:383:GLU:OE1	1:C:410:ARG:NE	2.37	0.46
1:C:525:LEU:O	1:C:530:ARG:NH1	2.48	0.46
1:C:596:ASP:HB2	1:C:602:GLN:HE21	1.80	0.46
2:A:134:CYS:HB2	2:A:148:TRP:CH2	2.51	0.46
1:C:447:HIS:HA	1:C:474:THR:O	2.15	0.46
3:B:208:LYS:N	3:B:209:PRO:HD2	2.30	0.46
2:A:161:GLU:HA	2:A:176:SER:O	2.15	0.46
3:B:155:GLU:HB3	3:B:156:PRO:HA	1.98	0.46
3:B:157:VAL:HG12	3:B:207:HIS:CD2	2.51	0.46
3:B:207:HIS:NE2	3:B:209:PRO:HG2	2.31	0.46
1:C:206:LYS:HZ2	1:C:224:GLY:HA2	1.80	0.46
3:B:202:ILE:HD12	3:B:216:LYS:C	2.36	0.45
1:C:206:LYS:HG2	1:C:212:ASP:HB3	1.97	0.45
2:A:118:PHE:HB2	2:A:133:VAL:CG1	2.47	0.45
2:A:185:ASP:N	2:A:185:ASP:OD1	2.50	0.44
3:B:43:LYS:HE3	3:B:43:LYS:HA	2.00	0.44
2:A:122:ASP:HA	2:A:125:LEU:HD12	2.00	0.44
1:C:41:THR:HA	1:C:65:ALA:O	2.18	0.44
1:C:434:ARG:HD2	1:C:504:THR:O	2.18	0.43
1:C:131:VAL:HG21	1:C:147:TRP:CE3	2.53	0.43
1:C:19:THR:HA	1:C:22:ASP:OD2	2.19	0.43
1:C:178:LYS:HD2	1:C:178:LYS:HA	1.72	0.43
3:B:6:GLU:HA	3:B:21:SER:O	2.18	0.43
1:C:294:PRO:HB2	1:C:297:ASN:ND2	2.34	0.42
2:A:146:VAL:HG12	2:A:196:VAL:HB	2.01	0.42
3:B:178:GLN:HG2	3:B:178:GLN:H	1.72	0.42
2:A:107:LYS:HA	2:A:140:TYR:OH	2.19	0.42
2:A:207:LYS:HE2	2:A:207:LYS:HB2	1.80	0.42
3:B:162:ASN:HD22	3:B:202:ILE:CG2	2.33	0.42
1:C:2:GLN:CB	1:C:32:GLN:HE21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ASP:OD1	1:C:143:ASP:N	2.52	0.42
2:A:131:SER:HA	2:A:179:LEU:O	2.20	0.42
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.87	0.41
1:C:209:LEU:O	1:C:212:ASP:HB2	2.20	0.41
2:A:211:ARG:HD2	2:A:211:ARG:HA	1.86	0.41
3:B:63:SER:O	3:B:67:ARG:NH1	2.53	0.41
1:C:340:GLN:CD	1:C:340:GLN:H	2.22	0.41
2:A:146:VAL:HG12	2:A:196:VAL:CG2	2.50	0.41
3:B:19:ARG:HB2	3:B:82:GLN:OE1	2.21	0.41
1:C:604:CYS:HA	1:C:605:PRO:HD3	1.90	0.41
2:A:118:PHE:HD2	2:A:133:VAL:HG13	1.85	0.41
2:A:145:LYS:O	2:A:196:VAL:HA	2.20	0.41
2:A:155:GLN:HB3	2:A:158:ASN:HD21	1.86	0.41
1:C:293:CYS:SG	1:C:299:GLU:HG2	2.61	0.40
3:B:161:TRP:CH2	3:B:203:CYS:HB3	2.57	0.40
1:C:300:VAL:HG21	1:C:310:GLU:CD	2.42	0.40
1:C:588:TYR:N	1:C:588:TYR:CD1	2.89	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	C	583/658 (89%)	559 (96%)	23 (4%)	1 (0%)	47 73
2	A	209/214 (98%)	202 (97%)	7 (3%)	0	100 100
3	B	206/231 (89%)	198 (96%)	8 (4%)	0	100 100
All	All	998/1103 (90%)	959 (96%)	38 (4%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	PRO

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	C	508/564 (90%)	501 (99%)	7 (1%)	67 86
2	A	187/189 (99%)	182 (97%)	5 (3%)	44 74
3	B	173/191 (91%)	171 (99%)	2 (1%)	71 88
All	All	868/944 (92%)	854 (98%)	14 (2%)	62 85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	THR
1	C	144	THR
1	C	148	LYS
1	C	227	HIS
1	C	396	SER
1	C	408	VAL
1	C	577	ARG
2	A	103	LYS
2	A	152	ASN
2	A	169	LYS
2	A	176	SER
2	A	185	ASP
3	B	151	ASP
3	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN
1	C	35	GLN
1	C	97	ASN

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Mol	Chain	Res	Type
1	C	191	GLN
1	C	217	GLN
1	C	235	HIS
1	C	340	GLN
1	C	449	ASN
1	C	491	GLN
2	A	27	GLN
2	A	37	GLN
2	A	38	GLN
2	A	124	GLN
3	B	112	GLN
3	B	162	ASN
3	B	178	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
4	NAG	C	701	1	14,14,15	1.14	2 (14%)	17,19,21	0.69	1 (5%)

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
4	NAG	C	701	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	701	NAG	O5-C1	3.40	1.49	1.43
4	C	701	NAG	C1-C2	2.49	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	701	NAG	C1-O5-C5	2.42	115.47	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	701	NAG	O5-C5-C6-O6
4	C	701	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	C	589/658 (89%)	0.08	8 (1%) 75 77	22, 50, 93, 134	0
2	A	211/214 (98%)	0.72	27 (12%) 3 3	39, 73, 144, 163	0
3	B	210/231 (90%)	0.64	29 (13%) 2 2	42, 81, 123, 145	0
All	All	1010/1103 (91%)	0.33	64 (6%) 20 19	22, 61, 127, 163	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	180	THR	5.1
2	A	127	SER	4.8
1	C	313	SER	4.6
2	A	181	LEU	4.6
3	B	148	LEU	4.4
2	A	209	PHE	4.2
2	A	135	LEU	4.1
2	A	129	THR	4.0
3	B	195	SER	3.8
3	B	217	LYS	3.8
3	B	149	VAL	3.7
2	A	128	GLY	3.7
3	B	206	ASN	3.6
3	B	201	TYR	3.6
2	A	1	ASP	3.5
2	A	179	LEU	3.5
3	B	185	LEU	3.4
3	B	152	TYR	3.4
3	B	202	ILE	3.3
3	B	214	VAL	3.2
2	A	118	PHE	3.1
3	B	145	LEU	3.1
1	C	315	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	133	VAL	3.0
2	A	117	ILE	3.0
2	A	211	ARG	3.0
2	A	178	THR	2.9
3	B	179	SER	2.9
2	A	125	LEU	2.9
3	B	178	GLN	2.9
2	A	192	TYR	2.9
1	C	311	LYS	2.9
3	B	205	VAL	2.9
3	B	182	LEU	2.7
2	A	184	ALA	2.7
2	A	186	TYR	2.7
3	B	132	ALA	2.7
3	B	157	VAL	2.7
2	A	154	LEU	2.6
3	B	183	TYR	2.6
2	A	123	GLU	2.5
3	B	151	ASP	2.5
1	C	285	ASP	2.5
3	B	133	PRO	2.5
3	B	129	PHE	2.5
2	A	148	TRP	2.5
3	B	200	THR	2.4
3	B	207	HIS	2.4
1	C	310	GLU	2.4
2	A	132	VAL	2.4
3	B	127	SER	2.3
2	A	187	GLU	2.2
1	C	282	LEU	2.2
2	A	121	SER	2.2
3	B	147	CYS	2.1
2	A	160	GLN	2.1
3	B	215	ASP	2.1
2	A	191	VAL	2.1
1	C	597	GLU	2.1
1	C	296	HIS	2.0
3	B	208	LYS	2.0
2	A	177	SER	2.0
3	B	184	SER	2.0
3	B	191	VAL	2.0

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)

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, 95^{th} 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
4	NAG	C	701	14/15	0.85	0.23	43,63,67,72	0

6.5 Other polymers (i)

There are no such residues in this entry.