



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:08 AM GMT

PDB ID : 1F0B  
Title : CRYSTAL STRUCTURE OF THE GREEN FLUORESCENT PROTEIN  
(GFP) VARIANT YFP-H148Q  
Authors : Wachter, R.M.; Yarbrough, D.; Kallio, K.; Remington, S.J.  
Deposited on : 2000-05-15  
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

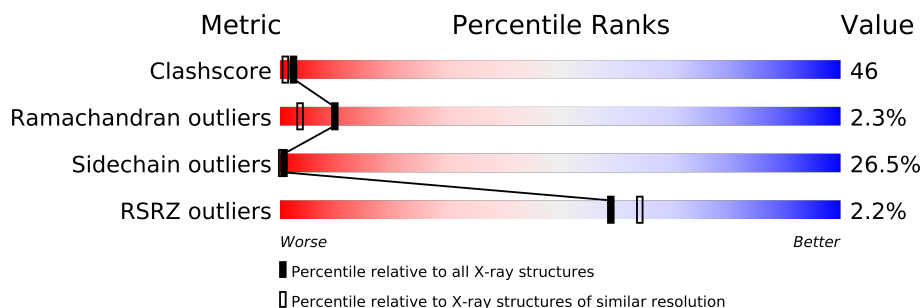
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1941 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	36	0	0
			1816	1159	306	345	6			

There are 8 discrepancies between the modelled and reference sequences:

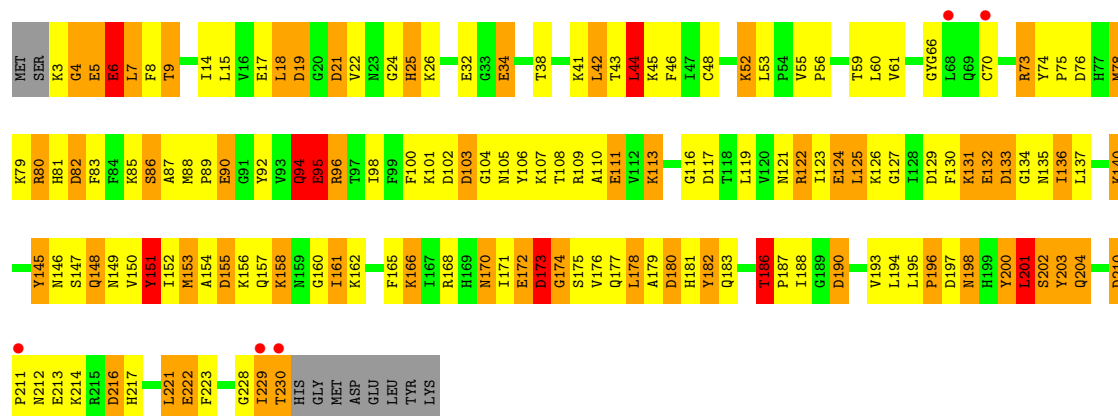
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CR2	SER	CHROMOPHORE	UNP P42212
A	66	CR2	TYR	CHROMOPHORE	UNP P42212
A	66	CR2	GLY	CHROMOPHORE	UNP P42212
A	68	LEU	VAL	ENGINEERED	UNP P42212
A	72	ALA	SER	ENGINEERED	UNP P42212
A	80	ARG	GLN	ENGINEERED	UNP P42212
A	148	GLN	HIS	ENGINEERED	UNP P42212
A	203	TYR	THR	ENGINEERED	UNP P42212

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		

i

• Molecule 1: GREEN FLUORESCENT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.66Å 62.65Å 66.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.50 – 2.10 22.46 – 2.04	Depositor EDS
% Data completeness (in resolution range)	81.5 (22.50-2.10) 80.3 (22.46-2.04)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.82 (at 2.04Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.188 , (Not available) 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 112.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 11402 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: CR2

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	1.31	15/1838 (0.8%)	1.79	55/2482 (2.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLU	CD-OE1	-7.39	1.17	1.25
1	A	222	GLU	CD-OE1	-7.12	1.17	1.25
1	A	5	GLU	CD-OE2	6.69	1.33	1.25
1	A	124	GLU	CD-OE2	6.52	1.32	1.25
1	A	34	GLU	CD-OE2	6.43	1.32	1.25
1	A	90	GLU	CD-OE2	6.35	1.32	1.25
1	A	132	GLU	CD-OE2	6.16	1.32	1.25
1	A	6	GLU	CD-OE2	5.96	1.32	1.25
1	A	17	GLU	CD-OE2	5.47	1.31	1.25
1	A	95	GLU	CD-OE2	5.46	1.31	1.25
1	A	111	GLU	CD-OE2	5.42	1.31	1.25
1	A	222	GLU	CD-OE2	5.32	1.31	1.25
1	A	172	GLU	CD-OE2	5.25	1.31	1.25
1	A	32	GLU	CD-OE2	5.14	1.31	1.25
1	A	213	GLU	CD-OE2	5.02	1.31	1.25

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	CB-CG-OD2	-9.06	110.14	118.30
1	A	173	ASP	CB-CG-OD1	8.93	126.34	118.30
1	A	102	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	A	210	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	A	106	TYR	CB-CG-CD1	8.74	126.24	121.00
1	A	102	ASP	CB-CG-OD1	8.14	125.62	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASP	CB-CG-OD1	8.12	125.61	118.30
1	A	82	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	21	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	21	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	103	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	180	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	106	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	A	82	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	129	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	216	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	19	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	155	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	155	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	96	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	76	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	129	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	173	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	44	LEU	CB-CA-C	-6.39	98.07	110.20
1	A	201	LEU	N-CA-CB	6.25	122.89	110.40
1	A	76	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	151	TYR	CB-CG-CD1	6.09	124.65	121.00
1	A	203	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	216	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	A	190	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	48	CYS	CA-CB-SG	-5.96	103.28	114.00
1	A	73	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	9	THR	N-CA-CB	-5.84	99.21	110.30
1	A	122	ARG	N-CA-CB	-5.78	100.19	110.60
1	A	186	THR	N-CA-CB	5.74	121.21	110.30
1	A	145	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	122	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	94	GLN	N-CA-CB	-5.61	100.50	110.60
1	A	180	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	182	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	42	LEU	CB-CA-C	-5.47	99.80	110.20
1	A	73	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	190	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	14	ILE	CB-CA-C	-5.36	100.89	111.60
1	A	92	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	122	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	197	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	116	GLY	N-CA-C	-5.21	100.08	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASP	C-N-CA	5.21	133.24	122.30
1	A	160	GLY	N-CA-C	-5.18	100.16	113.10
1	A	45	LYS	N-CA-CB	5.14	119.86	110.60
1	A	117	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	201	LEU	CB-CA-C	5.12	119.92	110.20
1	A	78	MET	CB-CA-C	-5.06	100.27	110.40
1	A	173	ASP	CA-CB-CG	5.05	124.51	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1816	0	1762	161	0
2	A	125	0	0	12	0
All	All	1941	0	1762	161	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 46.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:ASN:HD22	1:A:198:ASN:H	1.03	0.97
1:A:198:ASN:ND2	1:A:198:ASN:H	1.59	0.96
1:A:152:ILE:HD12	1:A:200:TYR:HA	1.51	0.91
1:A:7:LEU:HD12	1:A:7:LEU:H	1.33	0.91
1:A:135:ASN:HA	1:A:140:LYS:HG2	1.55	0.88
1:A:166:LYS:HG3	1:A:178:LEU:HD21	1.56	0.88
1:A:78:MET:HE1	1:A:229:ILE:H	1.40	0.86
1:A:146:ASN:HD21	1:A:170:ASN:HD21	1.19	0.86
1:A:135:ASN:HA	1:A:140:LYS:CG	2.05	0.86
1:A:108:THR:HG22	1:A:125:LEU:HB2	1.60	0.84
1:A:168:ARG:HB3	1:A:176:VAL:HG11	1.59	0.84

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:LYS:HG3	1:A:223:PHE:CE1	2.13	0.83
1:A:155:ASP:HB2	1:A:162:LYS:HG3	1.62	0.80
1:A:198:ASN:N	1:A:198:ASN:ND2	2.30	0.79
1:A:24:GLY:HA2	2:A:373:HOH:O	1.83	0.79
1:A:103:ASP:HA	1:A:131:LYS:HZ2	1.48	0.78
1:A:103:ASP:HA	1:A:131:LYS:NZ	2.01	0.76
1:A:22:VAL:HG22	1:A:127:GLY:HA3	1.67	0.75
1:A:7:LEU:HD12	1:A:7:LEU:N	2.01	0.74
1:A:221:LEU:HD11	1:A:223:PHE:CE2	2.23	0.72
1:A:75:PRO:HA	2:A:431:HOH:O	1.90	0.71
1:A:7:LEU:CD1	1:A:7:LEU:H	2.04	0.71
1:A:119:LEU:HD12	2:A:433:HOH:O	1.92	0.70
1:A:78:MET:HG2	1:A:229:ILE:HG21	1.73	0.70
1:A:155:ASP:CG	1:A:162:LYS:HE2	2.14	0.69
1:A:152:ILE:CD1	1:A:200:TYR:HA	2.23	0.68
1:A:86:SER:O	1:A:193:VAL:HG12	1.94	0.68
1:A:166:LYS:HD3	1:A:178:LEU:HD11	1.74	0.68
1:A:146:ASN:ND2	1:A:168:ARG:HH12	1.93	0.66
1:A:228:GLY:HA2	2:A:419:HOH:O	1.94	0.66
1:A:52:LYS:HE2	1:A:216:ASP:HB2	1.77	0.65
1:A:195:LEU:HD22	1:A:195:LEU:N	2.12	0.65
1:A:110:ALA:HB1	1:A:121:ASN:OD1	1.96	0.65
1:A:135:ASN:HA	1:A:140:LYS:HG3	1.78	0.65
1:A:78:MET:HG2	1:A:229:ILE:CG2	2.26	0.65
1:A:4:GLY:O	1:A:7:LEU:HD13	1.97	0.64
1:A:146:ASN:ND2	1:A:168:ARG:NH1	2.45	0.64
1:A:94:GLN:HG3	2:A:252:HOH:O	1.96	0.64
1:A:153:MET:HB2	1:A:198:ASN:OD1	1.98	0.64
1:A:146:ASN:ND2	1:A:170:ASN:HD21	1.94	0.64
1:A:146:ASN:HD22	1:A:168:ARG:NH1	1.96	0.63
1:A:104:GLY:HA2	2:A:284:HOH:O	1.97	0.63
1:A:55:VAL:HB	1:A:56:PRO:HD2	1.81	0.63
1:A:166:LYS:CD	1:A:178:LEU:HD11	2.29	0.63
1:A:155:ASP:OD2	1:A:158:LYS:HB2	1.98	0.63
1:A:125:LEU:HD12	1:A:126:LYS:N	2.14	0.62
1:A:178:LEU:HD22	1:A:179:ALA:N	2.15	0.62
1:A:146:ASN:HD21	1:A:170:ASN:ND2	1.94	0.62
1:A:178:LEU:HD22	1:A:179:ALA:H	1.65	0.61
1:A:148:GLN:HG3	1:A:149:ASN:N	2.16	0.61
1:A:70:CYS:O	1:A:85:LYS:HE3	2.01	0.60
1:A:151:TYR:CD2	1:A:200:TYR:CD1	2.89	0.60
1:A:21:ASP:OD2	1:A:26:LYS:HD3	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ARG:HB3	1:A:176:VAL:CG1	2.30	0.59
1:A:21:ASP:HA	1:A:25:HIS:O	2.02	0.59
1:A:171:ILE:HG22	1:A:173:ASP:H	1.68	0.59
1:A:89:PRO:HD2	1:A:90:GLU:OE2	2.02	0.59
1:A:130:PHE:HE2	1:A:136:ILE:HD13	1.67	0.59
1:A:204:GLN:HG3	2:A:365:HOH:O	2.03	0.59
1:A:78:MET:CE	1:A:229:ILE:H	2.13	0.58
1:A:152:ILE:HD11	1:A:201:LEU:HG	1.85	0.58
1:A:100:PHE:CG	1:A:136:ILE:HD11	2.37	0.58
1:A:151:TYR:N	1:A:151:TYR:CD1	2.72	0.57
1:A:52:LYS:HE3	1:A:52:LYS:N	2.19	0.57
1:A:4:GLY:HA2	1:A:7:LEU:HD13	1.85	0.57
1:A:43:THR:HB	2:A:400:HOH:O	2.05	0.57
1:A:46:PHE:O	1:A:217:HIS:HB2	2.03	0.57
1:A:173:ASP:C	1:A:175:SER:H	2.03	0.56
1:A:96:ARG:HA	1:A:182:TYR:O	2.06	0.56
1:A:173:ASP:O	1:A:175:SER:HB3	2.05	0.55
1:A:155:ASP:OD2	1:A:162:LYS:HE2	2.07	0.54
1:A:18:LEU:HD13	1:A:19:ASP:C	2.28	0.54
1:A:83:PHE:HB2	1:A:194:LEU:O	2.07	0.54
1:A:82:ASP:OD2	1:A:85:LYS:HG3	2.08	0.54
1:A:113:LYS:HE3	2:A:351:HOH:O	2.08	0.54
1:A:103:ASP:OD2	1:A:131:LYS:HE3	2.08	0.54
1:A:151:TYR:HD2	1:A:200:TYR:CD1	2.26	0.54
1:A:133:ASP:N	1:A:133:ASP:OD1	2.40	0.54
1:A:178:LEU:CD2	1:A:179:ALA:H	2.21	0.53
1:A:171:ILE:HG22	1:A:172:GLU:N	2.22	0.53
1:A:173:ASP:O	1:A:175:SER:N	2.26	0.53
1:A:74:TYR:O	1:A:79:LYS:HE2	2.07	0.53
1:A:151:TYR:HD2	1:A:200:TYR:HD1	1.57	0.53
1:A:173:ASP:O	1:A:173:ASP:OD1	2.26	0.52
1:A:172:GLU:O	1:A:174:GLY:N	2.43	0.52
1:A:165:PHE:O	1:A:181:HIS:HB2	2.10	0.52
1:A:154:ALA:HA	1:A:161:ILE:HG22	1.92	0.52
1:A:110:ALA:HB2	1:A:123:ILE:HG12	1.91	0.51
1:A:100:PHE:CD2	1:A:136:ILE:HD11	2.46	0.51
1:A:44:LEU:HB3	1:A:46:PHE:CE1	2.45	0.51
1:A:155:ASP:CG	1:A:158:LYS:HB2	2.31	0.51
1:A:122:ARG:NH2	2:A:346:HOH:O	2.44	0.51
1:A:165:PHE:O	1:A:181:HIS:N	2.32	0.50
1:A:103:ASP:HA	1:A:131:LYS:CE	2.41	0.50
1:A:119:LEU:C	1:A:119:LEU:HD13	2.32	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:18:LEU:HD13	1:A:19:ASP:N	2.26	0.50
1:A:75:PRO:O	1:A:79:LYS:HG2	2.12	0.49
1:A:80:ARG:HG3	2:A:317:HOH:O	2.13	0.49
1:A:4:GLY:CA	1:A:7:LEU:HD13	2.42	0.48
1:A:171:ILE:HG22	1:A:173:ASP:N	2.27	0.48
1:A:135:ASN:CA	1:A:140:LYS:HG2	2.36	0.48
1:A:61:VAL:O	1:A:66:CR2:HA11	2.13	0.48
1:A:56:PRO:HD2	1:A:136:ILE:HG23	1.95	0.48
1:A:103:ASP:CG	1:A:131:LYS:HD2	2.34	0.48
1:A:74:TYR:O	1:A:79:LYS:HD3	2.13	0.48
1:A:21:ASP:CG	1:A:26:LYS:HG2	2.34	0.48
1:A:6:GLU:H	1:A:6:GLU:HG3	1.43	0.47
1:A:175:SER:OG	1:A:176:VAL:N	2.47	0.47
1:A:4:GLY:HA2	1:A:7:LEU:CD1	2.45	0.47
1:A:229:ILE:O	1:A:230:THR:OG1	2.29	0.47
1:A:96:ARG:NE	1:A:183:GLN:OE1	2.48	0.47
1:A:81:HIS:CD2	1:A:229:ILE:HG12	2.50	0.47
1:A:123:ILE:HG22	1:A:124:GLU:N	2.29	0.47
1:A:53:LEU:HD21	1:A:60:LEU:CD1	2.45	0.47
1:A:147:SER:OG	1:A:148:GLN:N	2.47	0.46
1:A:149:ASN:ND2	1:A:202:SER:HB2	2.30	0.46
1:A:221:LEU:HD13	1:A:222:GLU:N	2.29	0.46
1:A:149:ASN:HD22	1:A:202:SER:HB2	1.80	0.46
1:A:53:LEU:HD21	1:A:60:LEU:HD12	1.98	0.46
1:A:166:LYS:HA	1:A:179:ALA:O	2.15	0.46
1:A:201:LEU:HD13	1:A:203:TYR:HE1	1.80	0.45
1:A:148:GLN:CG	1:A:149:ASN:N	2.80	0.45
1:A:155:ASP:HB2	1:A:162:LYS:CG	2.40	0.45
1:A:8:PHE:CZ	1:A:88:MET:HG3	2.52	0.45
1:A:130:PHE:CE2	1:A:136:ILE:HD13	2.51	0.45
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.79	0.45
1:A:4:GLY:C	1:A:7:LEU:HD13	2.38	0.44
1:A:151:TYR:CD2	1:A:200:TYR:HD1	2.31	0.44
1:A:18:LEU:HD13	1:A:19:ASP:O	2.18	0.43
1:A:181:HIS:N	1:A:181:HIS:ND1	2.66	0.43
1:A:150:VAL:HB	1:A:201:LEU:HD12	2.00	0.43
1:A:186:THR:OG1	1:A:187:PRO:HD2	2.18	0.43
1:A:150:VAL:CG1	1:A:201:LEU:CD1	2.97	0.43
1:A:38:THR:O	1:A:73:ARG:HD3	2.18	0.43
1:A:195:LEU:N	1:A:195:LEU:CD2	2.80	0.43
1:A:110:ALA:HB2	1:A:123:ILE:CG1	2.48	0.43
1:A:59:THR:HG22	1:A:100:PHE:CE2	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:73:ARG:HG2	1:A:73:ARG:O	2.18	0.42
1:A:178:LEU:CD2	1:A:179:ALA:N	2.80	0.42
1:A:130:PHE:HB3	1:A:137:LEU:HD12	2.01	0.42
1:A:221:LEU:CD1	1:A:223:PHE:CE2	2.97	0.42
1:A:95:GLU:O	1:A:183:GLN:HA	2.19	0.42
1:A:21:ASP:CB	1:A:26:LYS:HG2	2.49	0.42
1:A:176:VAL:CG1	1:A:177:GLN:N	2.79	0.42
1:A:55:VAL:HB	1:A:56:PRO:CD	2.48	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.48	0.41
1:A:85:LYS:C	1:A:87:ALA:H	2.23	0.41
1:A:103:ASP:OD2	1:A:104:GLY:N	2.48	0.41
1:A:171:ILE:CG2	1:A:172:GLU:N	2.83	0.41
1:A:88:MET:HB3	1:A:89:PRO:HA	2.01	0.41
1:A:229:ILE:HA	1:A:229:ILE:HD12	1.60	0.41
1:A:123:ILE:CG2	1:A:124:GLU:N	2.83	0.41
1:A:140:LYS:HD2	1:A:140:LYS:N	2.35	0.41
1:A:42:LEU:HG	2:A:425:HOH:O	2.21	0.41
1:A:210:ASP:OD1	1:A:211:PRO:HD2	2.21	0.41
1:A:81:HIS:ND1	1:A:196:PRO:HA	2.36	0.40
1:A:4:GLY:CA	1:A:7:LEU:CD1	2.99	0.40
1:A:166:LYS:CG	1:A:178:LEU:HD21	2.39	0.40
1:A:103:ASP:OD2	1:A:131:LYS:HD2	2.21	0.40
1:A:98:ILE:HG12	1:A:181:HIS:CD2	2.56	0.40
1:A:82:ASP:O	1:A:86:SER:HB3	2.21	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	221/236 (94%)	204 (92%)	12 (5%)	5 (2%)	10   3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	174	GLY
1	A	134	GLY
1	A	136	ILE
1	A	4	GLY

### 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	196/205 (96%)	144 (74%)	52 (26%)	<b>1</b> <b>0</b>

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	GLU
1	A	6	GLU
1	A	7	LEU
1	A	9	THR
1	A	15	LEU
1	A	18	LEU
1	A	25	HIS
1	A	34	GLU
1	A	44	LEU
1	A	52	LYS
1	A	80	ARG
1	A	86	SER
1	A	94	GLN
1	A	95	GLU
1	A	105	ASN
1	A	107	LYS
1	A	109	ARG
1	A	111	GLU
1	A	113	LYS
1	A	125	LEU
1	A	131	LYS
1	A	132	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	133	ASP
1	A	140	LYS
1	A	145	TYR
1	A	148	GLN
1	A	151	TYR
1	A	153	MET
1	A	156	LYS
1	A	157	GLN
1	A	158	LYS
1	A	161	ILE
1	A	166	LYS
1	A	170	ASN
1	A	173	ASP
1	A	178	LEU
1	A	180	ASP
1	A	186	THR
1	A	188	ILE
1	A	190	ASP
1	A	196	PRO
1	A	198	ASN
1	A	200	TYR
1	A	201	LEU
1	A	202	SER
1	A	204	GLN
1	A	212	ASN
1	A	214	LYS
1	A	221	LEU
1	A	229	ILE
1	A	230	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	105	ASN
1	A	139	HIS
1	A	146	ASN
1	A	149	ASN
1	A	170	ASN
1	A	198	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	CR2	A	66	1	20,20,21	4.74	10 (50%)	25,27,29	1.92	9 (36%)

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	CR2	A	66	1	-	1/8/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CR2	O3-C3	15.17	1.21	1.11
1	A	66	CR2	C1-N3	7.62	1.48	1.37
1	A	66	CR2	CA3-N3	-7.07	1.41	1.47
1	A	66	CR2	CG2-CB2	-5.57	1.35	1.46
1	A	66	CR2	CE1-CZ	4.62	1.48	1.38
1	A	66	CR2	OH-CZ	-4.25	1.26	1.37
1	A	66	CR2	CD1-CG2	2.84	1.44	1.39
1	A	66	CR2	CA3-C3	2.80	1.52	1.48
1	A	66	CR2	CE2-CZ	2.60	1.44	1.38
1	A	66	CR2	CA1-C1	2.52	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CR2	CG2-CB2-CA2	3.55	134.18	130.10
1	A	66	CR2	CA2-C2-N3	3.51	105.44	103.44
1	A	66	CR2	CA3-N3-C1	3.32	131.68	124.64
1	A	66	CR2	CA1-C1-N3	2.91	127.76	123.37
1	A	66	CR2	CB2-CA2-C2	-2.91	117.99	122.46
1	A	66	CR2	CA3-N3-C2	-2.87	121.68	123.46
1	A	66	CR2	C2-CA2-N2	2.31	110.66	108.91
1	A	66	CR2	CA2-N2-C1	2.30	107.67	105.81
1	A	66	CR2	CA1-C1-N2	-2.05	121.39	123.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CR2	N3-C1-CA1-N1

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/236 (95%)	0.01	5 (2%) 59 64	20, 32, 63, 88	11 (4%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ILE	3.1
1	A	230	THR	2.8
1	A	68	LEU	2.7
1	A	211	PRO	2.1
1	A	70	CYS	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CR2	A	66	19/20	0.17	0.85	12,26,53,57	0

### 6.3 Carbohydrates

There are no carbohydrates 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.