



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 08:19 AM EDT

PDB ID : 1F09  
Title : CRYSTAL STRUCTURE OF THE GREEN FLUORESCENT PROTEIN (GFP) VARIANT YFP-H148Q WITH TWO BOUND IODIDES  
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Deposited on : 2000-05-15  
Resolution : 2.14 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](mailto: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.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

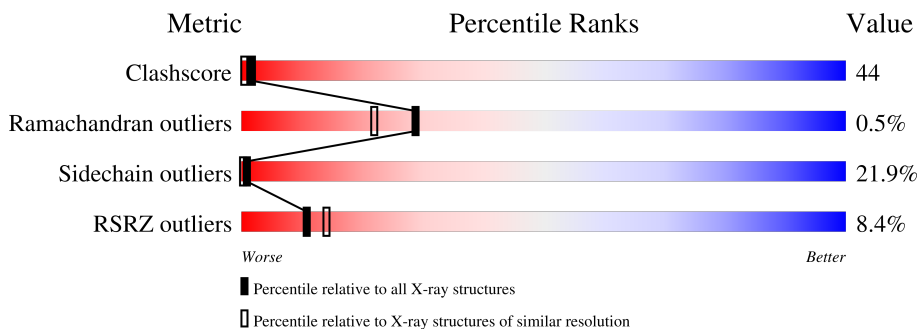
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 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	236	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1922 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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1815	1158	306	345	6	40	0	0

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 mutation	UNP P42212
A	72	ALA	SER	engineered mutation	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	148	GLN	HIS	engineered mutation	UNP P42212
A	203	TYR	THR	engineered mutation	UNP P42212

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	I 2	0	0

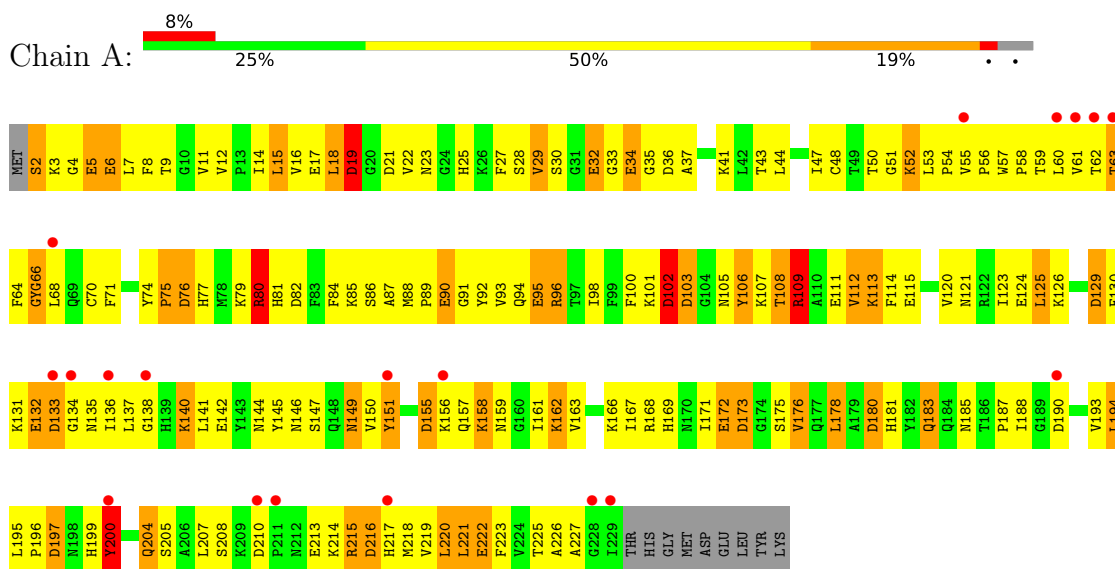
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total 105	O 105	0	0

### 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: GREEN FLUORESCENT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.20Å 62.82Å 68.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.10 – 2.14 30.13 – 2.14	Depositor EDS
% Data completeness (in resolution range)	85.6 (30.10-2.14) 85.3 (30.13-2.14)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.14Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.204 , (Not available) 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtrriage
Anisotropy	0.636	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 107.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: IOD, 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	1.17	16/1837 (0.9%)	1.70	48/2480 (1.9%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLU	CD-OE2	6.81	1.33	1.25
1	A	32	GLU	CD-OE2	6.76	1.33	1.25
1	A	222	GLU	CD-OE2	6.59	1.32	1.25
1	A	115	GLU	CD-OE2	6.55	1.32	1.25
1	A	90	GLU	CD-OE2	6.48	1.32	1.25
1	A	95	GLU	CD-OE2	6.31	1.32	1.25
1	A	17	GLU	CD-OE2	5.79	1.32	1.25
1	A	172	GLU	CD-OE2	5.78	1.32	1.25
1	A	142	GLU	CD-OE2	5.71	1.31	1.25
1	A	132	GLU	CD-OE2	5.46	1.31	1.25
1	A	17	GLU	CD-OE1	-5.43	1.19	1.25
1	A	213	GLU	CD-OE2	5.27	1.31	1.25
1	A	6	GLU	CD-OE2	5.25	1.31	1.25
1	A	142	GLU	CD-OE1	-5.19	1.20	1.25
1	A	34	GLU	CD-OE2	5.18	1.31	1.25
1	A	124	GLU	CD-OE2	5.14	1.31	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	CB-CG-OD2	-11.18	108.24	118.30
1	A	82	ASP	CB-CG-OD1	9.78	127.11	118.30
1	A	96	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	A	80	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	76	ASP	CB-CG-OD2	-8.14	110.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	TYR	CB-CG-CD1	7.72	125.63	121.00
1	A	200	TYR	CB-CA-C	-7.70	95.00	110.40
1	A	216	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	19	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	180	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	A	96	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	109	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	103	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	200	TYR	CA-CB-CG	6.92	126.55	113.40
1	A	21	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	15	LEU	N-CA-CB	-6.65	97.10	110.40
1	A	102	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	216	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	210	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	155	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	215	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	21	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	190	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	197	ASP	CB-CA-C	6.15	122.70	110.40
1	A	106	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	133	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	76	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	80	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	129	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	36	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	200	TYR	N-CA-CB	5.67	120.80	110.60
1	A	129	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	75	PRO	N-CA-CB	5.62	110.05	103.30
1	A	210	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	A	190	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	197	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	103	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	180	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	133	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	15	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	A	200	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	108	THR	CA-CB-CG2	-5.14	105.20	112.40
1	A	222	GLU	CB-CA-C	-5.12	100.17	110.40
1	A	197	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	173	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	155	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	200	TYR	CA-C-N	-5.04	106.10	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ALA	CB-CA-C	5.02	117.62	110.10

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	1815	0	1760	153	0
2	A	2	0	0	0	0
3	A	105	0	0	12	0
All	All	1922	0	1760	153	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 44.

All (153) 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:A:135:ASN:HA	1:A:140:LYS:HD3	1.23	1.19
1:A:4:GLY:HA2	1:A:7:LEU:HD13	1.43	0.99
1:A:18:LEU:HD12	1:A:19:ASP:N	1.83	0.92
1:A:220:LEU:HD11	1:A:222:GLU:HG2	1.53	0.91
1:A:161:ILE:HG13	1:A:185:ASN:HB2	1.53	0.88
1:A:96:ARG:HB2	1:A:108:THR:HG22	1.56	0.86
1:A:88:MET:CE	1:A:91:GLY:HA2	2.06	0.86
1:A:8:PHE:CE1	1:A:85:LYS:HG2	2.12	0.85
1:A:135:ASN:HA	1:A:140:LYS:CD	2.06	0.84
1:A:86:SER:HB3	1:A:194:LEU:HB2	1.60	0.83
1:A:86:SER:CB	1:A:194:LEU:HB2	2.08	0.83
1:A:52:LYS:N	1:A:52:LYS:HD2	1.94	0.82
1:A:75:PRO:HB2	1:A:77:HIS:CE1	2.15	0.81
1:A:18:LEU:HD11	1:A:125:LEU:HB2	1.63	0.81
1:A:156:LYS:O	1:A:157:GLN:C	2.16	0.81
1:A:81:HIS:CE1	1:A:197:ASP:H	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HB2	1:A:108:THR:CG2	2.11	0.78
1:A:141:LEU:HD13	1:A:169:HIS:HB3	1.62	0.78
1:A:141:LEU:HD13	1:A:169:HIS:CB	2.13	0.78
1:A:140:LYS:O	1:A:172:GLU:HG2	1.85	0.77
1:A:131:LYS:O	1:A:137:LEU:HB2	1.84	0.76
1:A:15:LEU:HD12	1:A:120:VAL:HG22	1.66	0.76
1:A:220:LEU:HD11	1:A:222:GLU:CG	2.17	0.73
1:A:14:ILE:HG21	1:A:44:LEU:HD21	1.71	0.73
1:A:108:THR:HG21	3:A:255:HOH:O	1.89	0.72
1:A:4:GLY:HA2	1:A:7:LEU:CD1	2.20	0.71
1:A:171:ILE:HG22	1:A:173:ASP:H	1.56	0.70
1:A:111:GLU:HG2	1:A:188:ILE:HD11	1.72	0.70
1:A:204:GLN:HB2	3:A:365:HOH:O	1.91	0.70
1:A:80:ARG:HG2	3:A:317:HOH:O	1.92	0.68
1:A:33:GLY:HA3	1:A:43:THR:O	1.94	0.67
1:A:88:MET:HE1	1:A:91:GLY:HA2	1.75	0.67
1:A:150:VAL:O	1:A:200:TYR:HB3	1.95	0.66
1:A:216:ASP:HA	3:A:269:HOH:O	1.95	0.66
1:A:136:ILE:HB	3:A:258:HOH:O	1.94	0.66
1:A:87:ALA:O	1:A:90:GLU:HB2	1.97	0.65
1:A:28:SER:HB2	1:A:50:THR:HG23	1.77	0.65
1:A:8:PHE:CD1	1:A:85:LYS:HD3	2.32	0.65
1:A:193:VAL:HG23	1:A:195:LEU:CD2	2.27	0.64
1:A:4:GLY:O	1:A:5:GLU:C	2.33	0.64
1:A:101:LYS:NZ	3:A:265:HOH:O	2.30	0.63
1:A:149:ASN:ND2	3:A:336:HOH:O	2.30	0.63
1:A:70:CYS:O	1:A:85:LYS:HE3	1.98	0.63
1:A:146:ASN:HB3	3:A:367:HOH:O	1.98	0.63
1:A:75:PRO:HA	3:A:315:HOH:O	1.97	0.63
1:A:215:ARG:O	1:A:217:HIS:ND1	2.29	0.62
1:A:151:TYR:CE2	1:A:200:TYR:HE1	2.16	0.62
1:A:88:MET:HE2	1:A:91:GLY:HA2	1.80	0.62
1:A:95:GLU:HA	1:A:108:THR:O	2.00	0.62
1:A:221:LEU:HD12	1:A:222:GLU:N	2.14	0.62
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.81	0.61
1:A:96:ARG:CB	1:A:108:THR:HG22	2.29	0.61
1:A:4:GLY:CA	1:A:7:LEU:HD13	2.23	0.61
1:A:18:LEU:HD12	1:A:19:ASP:H	1.62	0.60
1:A:144:ASN:HB2	3:A:298:HOH:O	2.01	0.60
1:A:93:VAL:O	1:A:185:ASN:HA	2.02	0.59
1:A:133:ASP:HA	3:A:325:HOH:O	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG22	1:A:64:PHE:N	2.17	0.59
1:A:134:GLY:O	1:A:138:GLY:HA3	2.03	0.58
1:A:58:PRO:HA	1:A:61:VAL:HG23	1.84	0.58
1:A:22:VAL:O	1:A:25:HIS:HB2	2.03	0.58
1:A:134:GLY:O	1:A:140:LYS:HD2	2.04	0.58
1:A:187:PRO:HG3	1:A:193:VAL:HG11	1.86	0.58
1:A:171:ILE:HD13	1:A:175:SER:HB3	1.87	0.57
1:A:92:TYR:CE1	1:A:112:VAL:HG13	2.39	0.57
1:A:193:VAL:HG23	1:A:195:LEU:HD22	1.85	0.57
1:A:167:ILE:HB	1:A:181:HIS:HE1	1.69	0.56
1:A:18:LEU:HD13	1:A:123:ILE:HG22	1.87	0.56
1:A:55:VAL:HB	1:A:56:PRO:CD	2.36	0.56
1:A:130:PHE:HB3	1:A:137:LEU:HG	1.86	0.56
1:A:207:LEU:HA	1:A:219:VAL:O	2.06	0.56
1:A:113:LYS:HD3	1:A:114:PHE:O	2.06	0.55
1:A:81:HIS:ND1	1:A:197:ASP:N	2.48	0.54
1:A:11:VAL:HG12	1:A:11:VAL:O	2.07	0.54
1:A:58:PRO:HA	1:A:61:VAL:CG2	2.37	0.54
1:A:171:ILE:HG22	1:A:172:GLU:N	2.22	0.54
1:A:94:GLN:OE1	1:A:183:GLN:NE2	2.41	0.54
1:A:158:LYS:O	1:A:159:ASN:C	2.46	0.54
1:A:96:ARG:CG	1:A:183:GLN:HB2	2.38	0.53
1:A:155:ASP:OD2	1:A:158:LYS:HB2	2.08	0.53
1:A:151:TYR:CD1	1:A:151:TYR:N	2.75	0.53
1:A:163:VAL:HB	1:A:183:GLN:HG2	1.90	0.53
1:A:88:MET:HE1	1:A:112:VAL:O	2.08	0.53
1:A:7:LEU:HD12	1:A:7:LEU:N	2.24	0.52
1:A:53:LEU:HG	1:A:54:PRO:HD2	1.90	0.52
1:A:221:LEU:HD12	1:A:221:LEU:C	2.30	0.52
1:A:171:ILE:HD12	1:A:176:VAL:N	2.25	0.52
1:A:175:SER:OG	1:A:176:VAL:N	2.43	0.51
1:A:151:TYR:CE2	1:A:200:TYR:CE1	2.97	0.51
1:A:8:PHE:CD1	1:A:85:LYS:HG2	2.44	0.51
1:A:27:PHE:CD2	1:A:54:PRO:HG2	2.46	0.51
1:A:167:ILE:O	1:A:178:LEU:HD22	2.11	0.50
1:A:47:ILE:HD12	3:A:270:HOH:O	2.11	0.50
1:A:100:PHE:CZ	1:A:106:TYR:CE2	3.00	0.50
1:A:29:VAL:HA	1:A:47:ILE:O	2.12	0.49
1:A:76:ASP:HA	1:A:79:LYS:HE3	1.95	0.48
1:A:57:TRP:CZ2	1:A:217:HIS:HA	2.48	0.48
1:A:12:VAL:HB	1:A:71:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:CYS:HB3	1:A:51:GLY:O	2.14	0.48
1:A:88:MET:HA	1:A:89:PRO:C	2.33	0.48
1:A:41:LYS:HG3	1:A:223:PHE:CE1	2.49	0.47
1:A:53:LEU:N	1:A:216:ASP:OD1	2.32	0.47
1:A:74:TYR:HA	1:A:226:ALA:HB3	1.95	0.47
1:A:56:PRO:O	1:A:59:THR:HG23	2.14	0.47
1:A:98:ILE:O	1:A:105:ASN:HA	2.14	0.47
1:A:70:CYS:HA	1:A:84:PHE:HB3	1.96	0.47
1:A:81:HIS:O	1:A:196:PRO:HB3	2.15	0.47
1:A:95:GLU:HG3	1:A:109:ARG:HG3	1.97	0.47
1:A:95:GLU:CG	1:A:109:ARG:HG3	2.45	0.47
1:A:149:ASN:ND2	1:A:149:ASN:N	2.61	0.47
1:A:130:PHE:HB3	1:A:137:LEU:CD1	2.45	0.46
1:A:130:PHE:CB	1:A:137:LEU:HD11	2.46	0.46
1:A:171:ILE:HD12	1:A:175:SER:C	2.35	0.46
1:A:89:PRO:O	1:A:90:GLU:C	2.54	0.46
1:A:12:VAL:O	1:A:34:GLU:HA	2.16	0.46
1:A:168:ARG:HG2	1:A:178:LEU:HD23	1.98	0.46
1:A:58:PRO:O	1:A:61:VAL:HG23	2.16	0.46
1:A:14:ILE:CG2	1:A:44:LEU:HD21	2.45	0.46
1:A:35:GLY:HA3	1:A:71:PHE:CD1	2.51	0.46
1:A:167:ILE:HB	1:A:181:HIS:CE1	2.50	0.45
1:A:81:HIS:CE1	1:A:197:ASP:HB2	2.51	0.45
1:A:130:PHE:HB2	1:A:137:LEU:HD11	1.98	0.45
1:A:199:HIS:HB2	1:A:227:ALA:O	2.17	0.44
1:A:2:SER:HB3	1:A:5:GLU:H	1.82	0.44
1:A:16:VAL:HG22	1:A:121:ASN:HB3	2.00	0.44
1:A:167:ILE:HD13	1:A:167:ILE:HA	1.77	0.44
1:A:168:ARG:HG2	1:A:178:LEU:CD2	2.48	0.44
1:A:171:ILE:CG2	1:A:172:GLU:N	2.80	0.44
1:A:56:PRO:HB2	1:A:59:THR:HG23	2.00	0.43
1:A:102:ASP:O	1:A:131:LYS:NZ	2.38	0.43
1:A:35:GLY:HA3	1:A:71:PHE:CE1	2.53	0.43
1:A:57:TRP:HB3	1:A:218:MET:SD	2.57	0.43
1:A:62:THR:HG22	1:A:66:CR2:CD1	2.49	0.43
1:A:151:TYR:CD2	1:A:200:TYR:CE1	3.07	0.43
1:A:163:VAL:O	1:A:183:GLN:N	2.51	0.43
1:A:100:PHE:CE1	1:A:106:TYR:CD2	3.07	0.43
1:A:2:SER:HB3	1:A:5:GLU:N	2.34	0.43
1:A:75:PRO:CB	1:A:77:HIS:CE1	2.97	0.42
1:A:155:ASP:HB2	1:A:162:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HB	1:A:71:PHE:CE1	2.55	0.42
1:A:81:HIS:CE1	1:A:197:ASP:N	2.78	0.42
1:A:108:THR:O	1:A:108:THR:HG23	2.20	0.42
1:A:48:CYS:SG	1:A:51:GLY:O	2.78	0.41
1:A:111:GLU:HG2	1:A:188:ILE:CD1	2.45	0.41
1:A:23:ASN:HD21	1:A:130:PHE:N	2.19	0.41
1:A:70:CYS:CA	1:A:84:PHE:HB3	2.50	0.41
1:A:53:LEU:HD21	1:A:60:LEU:HD11	2.02	0.41
1:A:18:LEU:HD22	1:A:123:ILE:HG21	2.02	0.41
1:A:57:TRP:CB	1:A:58:PRO:CD	2.99	0.40
1:A:51:GLY:C	1:A:52:LYS:HD2	2.39	0.40
1:A:62:THR:HG22	1:A:66:CR2:CG2	2.52	0.40
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.87	0.40
1:A:149:ASN:O	1:A:151:TYR:CE1	2.75	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	221/236 (94%)	206 (93%)	14 (6%)	1 (0%)	29 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	THR

### 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	196/205 (96%)	153 (78%)	43 (22%)	1 0

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LYS
1	A	6	GLU
1	A	18	LEU
1	A	19	ASP
1	A	29	VAL
1	A	30	SER
1	A	32	GLU
1	A	52	LYS
1	A	63	THR
1	A	68	LEU
1	A	80	ARG
1	A	102	ASP
1	A	103	ASP
1	A	107	LYS
1	A	109	ARG
1	A	112	VAL
1	A	113	LYS
1	A	125	LEU
1	A	126	LYS
1	A	129	ASP
1	A	132	GLU
1	A	140	LYS
1	A	145	TYR
1	A	147	SER
1	A	149	ASN
1	A	151	TYR
1	A	158	LYS
1	A	162	LYS
1	A	166	LYS
1	A	176	VAL
1	A	178	LEU
1	A	180	ASP
1	A	183	GLN

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	200	TYR
1	A	204	GLN
1	A	205	SER
1	A	208	SER
1	A	214	LYS
1	A	220	LEU
1	A	221	LEU
1	A	225	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	149	ASN
1	A	181	HIS

### 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	CR2	A	66	1	20,20,21	2.86	10 (50%)	25,27,29	2.58	8 (32%)

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	-	0/6/25/26	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	OH-CZ	-5.46	1.24	1.37
1	A	66	CR2	C1-N3	5.42	1.45	1.37
1	A	66	CR2	CG2-CB2	-4.99	1.37	1.46
1	A	66	CR2	CE1-CZ	4.13	1.46	1.38
1	A	66	CR2	CE2-CZ	3.97	1.46	1.38
1	A	66	CR2	CB2-CA2	3.46	1.38	1.35
1	A	66	CR2	CA2-C2	-3.20	1.45	1.48
1	A	66	CR2	CA2-N2	2.71	1.44	1.38
1	A	66	CR2	CD1-CG2	2.08	1.43	1.39
1	A	66	CR2	CD2-CG2	2.01	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CR2	CB2-CA2-C2	-5.85	115.29	122.28
1	A	66	CR2	CA2-C2-N3	5.80	106.11	103.37
1	A	66	CR2	C2-N3-C1	-5.39	105.36	107.99
1	A	66	CR2	CB2-CA2-N2	4.25	134.71	128.83
1	A	66	CR2	O2-C2-CA2	-3.73	128.87	130.96
1	A	66	CR2	CG2-CB2-CA2	2.90	133.50	129.94
1	A	66	CR2	CE2-CZ-CE1	-2.54	115.49	119.77
1	A	66	CR2	O3-C3-CA3	-2.51	118.81	126.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CR2	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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<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	225/236 (95%)	0.49	19 (8%) <b>11</b> <b>14</b>	17, 34, 56, 76	12 (5%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ILE	4.9
1	A	228	GLY	4.8
1	A	133	ASP	3.7
1	A	190	ASP	2.6
1	A	210	ASP	2.6
1	A	61	VAL	2.6
1	A	151	TYR	2.6
1	A	200	TYR	2.5
1	A	68	LEU	2.5
1	A	60	LEU	2.4
1	A	62	THR	2.3
1	A	55	VAL	2.3
1	A	211	PRO	2.2
1	A	134	GLY	2.2
1	A	217	HIS	2.2
1	A	63	THR	2.2
1	A	138	GLY	2.2
1	A	156	LYS	2.1
1	A	136	ILE	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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CR2	A	66	19/20	0.91	0.23	29,37,56,56	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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	A	251	1/1	0.98	0.12	39,39,39,39	1
2	IOD	A	254	1/1	1.00	0.15	30,30,30,30	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.