



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:02 PM GMT

PDB ID : 2DD9  
Title : A mutant of GFP-like protein from Chiridius poppei  
Authors : Suto, K.; Masuda, H.; Takenaka, Y.; Mizuno, H.  
Deposited on : 2006-01-24  
Resolution : 2.30 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>

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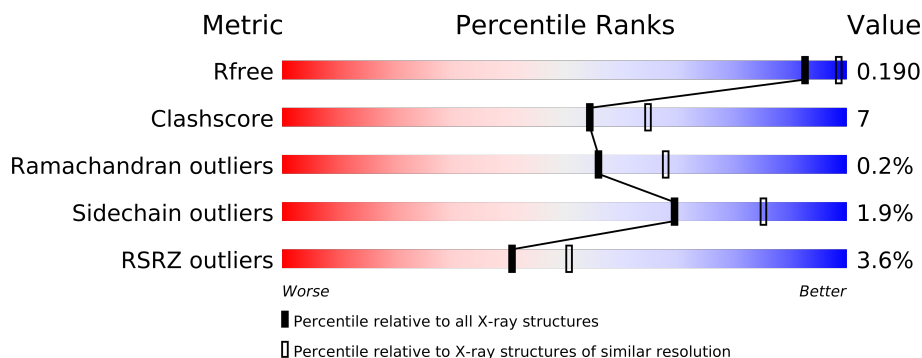
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	216	
1	B	216	
1	C	216	
1	D	216	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CXS	B	1001	-	X
2	CXS	B	1002	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7436 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.

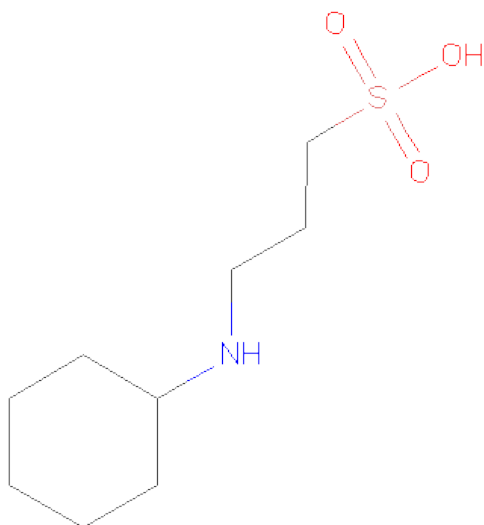
- Molecule 1 is a protein called green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1721	1099	288	325	9			
1	B	215	Total	C	N	O	S	0	0	0
			1721	1099	288	325	9			
1	C	214	Total	C	N	O	S	0	0	0
			1713	1095	287	322	9			
1	D	215	Total	C	N	O	S	0	0	0
			1721	1099	288	325	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	THR	HIS	ENGINEERED	UNP Q2MHN7
A	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
A	56	CR2	TYR	CHROMOPHORE	UNP Q2MHN7
A	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
B	52	THR	HIS	ENGINEERED	UNP Q2MHN7
B	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
B	56	CR2	TYR	CHROMOPHORE	UNP Q2MHN7
B	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
C	52	THR	HIS	ENGINEERED	UNP Q2MHN7
C	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
C	56	CR2	TYR	CHROMOPHORE	UNP Q2MHN7
C	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
D	52	THR	HIS	ENGINEERED	UNP Q2MHN7
D	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7
D	56	CR2	TYR	CHROMOPHORE	UNP Q2MHN7
D	56	CR2	GLY	CHROMOPHORE	UNP Q2MHN7

- Molecule 2 is 3-CYCLOHEXYL-1-PROPYLSULFONICACID (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	126	Total	O	0	0
			126	126		
4	C	101	Total	O	0	0
			101	101		

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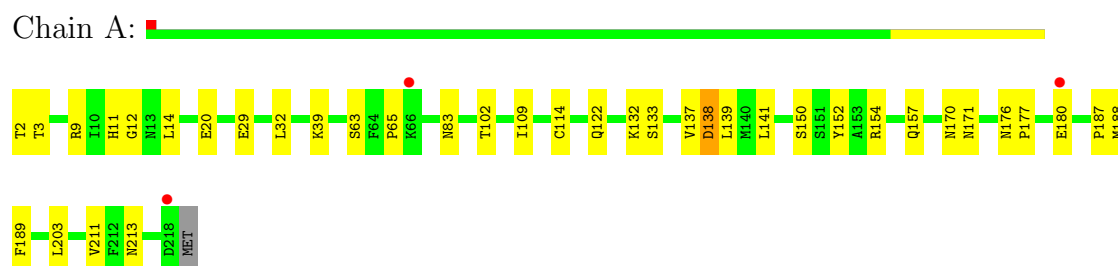
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	126	Total 126	O 126	0	0

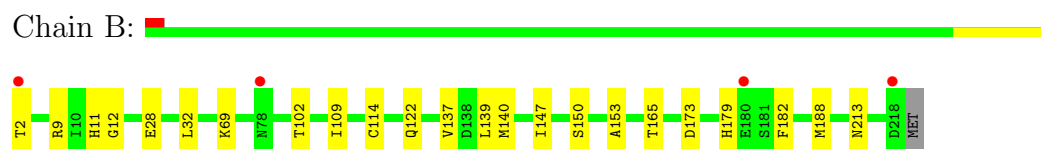
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

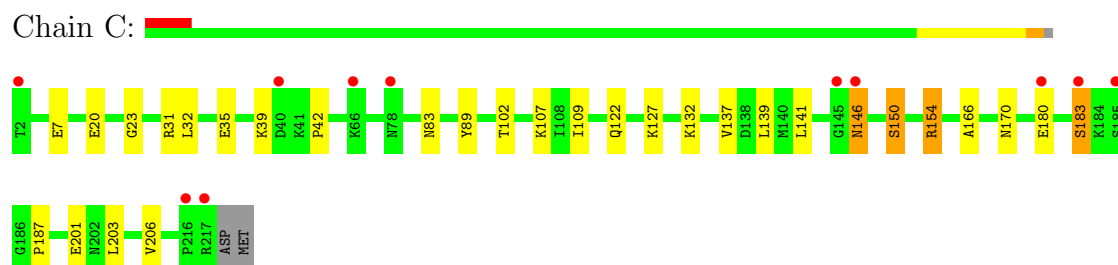
- Molecule 1: green fluorescent protein



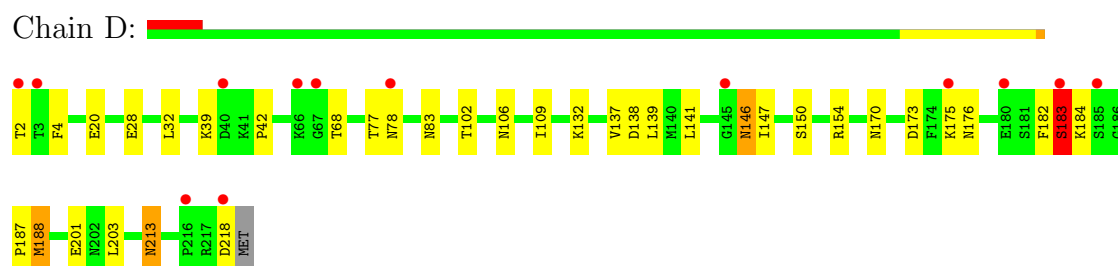
- Molecule 1: green fluorescent protein



- Molecule 1: green fluorescent protein



- 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, $\alpha$ , $\beta$ , $\gamma$	108.75Å 113.99Å 133.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.30 35.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.81-2.30) 100.0 (35.06-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.55 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.218 0.187 , 0.190	Depositor DCC
$R_{free}$ test set	3736 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 28.9	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74232 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.99 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8915e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, CXS, CL

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	0.46	0/1743	0.70	0/2347
1	B	0.48	0/1743	0.69	0/2347
1	C	0.44	0/1735	0.69	0/2336
1	D	0.45	0/1743	0.69	0/2347
All	All	0.46	0/6964	0.69	0/9377

There are no bond length outliers.

There are no bond angle outliers.

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	1721	0	1663	28	0
1	B	1721	0	1663	17	0
1	C	1713	0	1659	20	0
1	D	1721	0	1663	30	1
2	A	14	0	19	2	0
2	B	42	0	57	2	0
2	D	14	0	19	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	136	0	0	1	0
4	B	126	0	0	1	1
4	C	101	0	0	0	0
4	D	126	0	0	3	0
All	All	7436	0	6743	93	1

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 7.

All (93) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:VAL:HG11	1:B:137:VAL:HG11	1.63	0.81
1:C:7:GLU:HG3	1:C:107:LYS:HD2	1.68	0.76
1:B:2:THR:O	1:B:28:GLU:HA	1.90	0.72
1:C:137:VAL:HG11	1:D:137:VAL:HG11	1.73	0.70
1:D:146:ASN:HD22	1:D:146:ASN:H	1.37	0.70
1:B:139:LEU:HD23	1:B:140:MET:N	2.08	0.68
1:A:138:ASP:HB2	1:A:152:TYR:CD2	2.31	0.66
1:A:20:GLU:OE2	1:A:39:LYS:HE2	1.97	0.65
1:C:146:ASN:HD22	1:C:146:ASN:H	1.44	0.64
1:C:154:ARG:HH11	1:C:154:ARG:HB2	1.62	0.64
1:A:139:LEU:HD11	1:A:187:PRO:HB2	1.80	0.64
1:A:141:LEU:HD23	1:A:187:PRO:HB3	1.80	0.63
1:B:139:LEU:HD23	1:B:139:LEU:C	2.19	0.63
1:A:139:LEU:HD11	1:A:187:PRO:CB	2.30	0.62
1:D:154:ARG:HG3	1:D:154:ARG:HH11	1.65	0.61
1:C:154:ARG:NH1	1:C:154:ARG:HB2	2.15	0.60
1:A:139:LEU:CD1	1:A:187:PRO:HB2	2.31	0.60
1:D:32:LEU:HD12	1:D:32:LEU:C	2.24	0.58
1:A:83:ASN:HD21	1:A:170:ASN:HB3	1.69	0.58
1:A:141:LEU:CD2	1:A:187:PRO:HB3	2.36	0.55
1:B:69:LYS:HD3	1:B:179:HIS:CD2	2.42	0.55
1:B:153:ALA:HB1	2:B:1001:CXS:H81	1.88	0.55
1:D:2:THR:O	1:D:28:GLU:HA	2.08	0.54
1:A:32:LEU:C	1:A:32:LEU:HD12	2.27	0.54
1:D:141:LEU:HD23	1:D:187:PRO:HB3	1.90	0.54
1:C:20:GLU:OE1	1:C:39:LYS:HD3	2.09	0.53
1:B:147:ILE:HD13	1:B:173:ASP:HA	1.91	0.52
1:D:139:LEU:O	1:D:150:SER:HA	2.10	0.52
1:B:165:THR:HB	2:B:1001:CXS:H82	1.92	0.51
1:D:147:ILE:HD13	1:D:173:ASP:HA	1.92	0.51
1:A:188:MET:CE	1:A:213:ASN:HB3	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:203:LEU:HD12	1:D:203:LEU:N	2.26	0.51
1:A:29:GLU:HG3	1:A:63:SER:HA	1.92	0.51
1:D:20:GLU:OE1	1:D:39:LYS:HD3	2.11	0.50
1:A:132:LYS:HE2	1:A:157:GLN:OE1	2.12	0.50
1:C:32:LEU:C	1:C:32:LEU:HD12	2.32	0.50
1:C:154:ARG:HH11	1:C:154:ARG:CB	2.24	0.50
2:A:1003:CXS:H71	1:C:127:LYS:HA	1.93	0.50
1:B:32:LEU:HD12	1:B:32:LEU:C	2.32	0.49
1:A:138:ASP:OD1	1:A:150:SER:HB2	2.13	0.49
1:D:77:THR:O	1:D:77:THR:HG22	2.12	0.48
1:A:9:ARG:NH1	1:A:11:HIS:CD2	2.81	0.48
1:A:65:PRO:HD3	1:A:211:VAL:O	2.13	0.48
1:D:150:SER:OG	1:D:170:ASN:HB2	2.13	0.48
1:B:122:GLN:NE2	4:B:1155:HOH:O	2.46	0.48
1:A:139:LEU:HD13	1:A:189:PHE:CE2	2.48	0.48
1:A:171:ASN:HB3	2:A:1003:CXS:H82	1.95	0.48
1:D:78:ASN:O	1:D:176:ASN:ND2	2.42	0.47
1:C:146:ASN:N	1:C:146:ASN:HD22	2.08	0.47
1:C:83:ASN:HD21	1:C:170:ASN:HB3	1.79	0.47
1:A:133:SER:HB3	1:A:154:ARG:NH2	2.30	0.47
1:D:182:PHE:O	1:D:184:LYS:HD3	2.15	0.47
1:D:146:ASN:HD22	1:D:146:ASN:N	2.05	0.47
1:C:203:LEU:HD12	1:C:203:LEU:N	2.29	0.46
1:C:122:GLN:HE22	1:C:127:LYS:HZ1	1.63	0.46
1:A:12:GLY:HA3	1:A:114:CYS:O	2.16	0.46
1:B:139:LEU:CD2	1:B:139:LEU:C	2.85	0.45
1:A:176:ASN:HB3	1:A:177:PRO:HD2	1.99	0.45
1:A:203:LEU:N	1:A:203:LEU:HD12	2.31	0.45
1:B:12:GLY:HA3	1:B:114:CYS:O	2.17	0.45
1:D:175:LYS:HD3	1:D:175:LYS:O	2.17	0.45
1:D:213:ASN:C	1:D:213:ASN:HD22	2.20	0.45
1:D:83:ASN:HD21	1:D:170:ASN:HB3	1.82	0.45
1:C:141:LEU:HD23	1:C:187:PRO:HB3	1.98	0.44
1:A:138:ASP:HA	1:A:152:TYR:HB3	1.99	0.44
1:A:122:GLN:NE2	4:A:1363:HOH:O	2.49	0.44
1:D:102:THR:OG1	1:D:109:ILE:HB	2.17	0.44
1:D:42:PRO:HB3	1:D:201:GLU:HG2	2.00	0.44
1:A:102:THR:OG1	1:A:109:ILE:HB	2.18	0.44
1:A:188:MET:HE2	1:A:213:ASN:HB3	1.99	0.43
1:C:42:PRO:HB3	1:C:201:GLU:CG	2.47	0.43
1:C:102:THR:OG1	1:C:109:ILE:HB	2.18	0.43
1:D:138:ASP:OD1	1:D:150:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:154:ARG:HG3	1:D:154:ARG:NH1	2.33	0.43
1:A:139:LEU:O	1:A:150:SER:HA	2.19	0.42
1:D:182:PHE:O	1:D:183:SER:C	2.57	0.42
1:C:89:TYR:CD2	1:C:166:ALA:HB2	2.54	0.42
1:C:139:LEU:O	1:C:150:SER:HA	2.20	0.42
1:D:102:THR:HG23	4:D:1138:HOH:O	2.19	0.42
1:B:9:ARG:NH1	1:B:11:HIS:CD2	2.88	0.42
1:D:154:ARG:NH1	4:D:1110:HOH:O	2.46	0.42
1:D:132:LYS:NZ	4:D:1481:HOH:O	2.50	0.42
1:A:2:THR:HG23	1:A:3:THR:N	2.35	0.41
1:B:102:THR:OG1	1:B:109:ILE:HB	2.19	0.41
1:D:4:PHE:CD1	1:D:4:PHE:N	2.88	0.41
1:B:139:LEU:O	1:B:150:SER:HA	2.20	0.41
1:B:188:MET:HG2	1:B:213:ASN:HB3	2.03	0.41
1:D:42:PRO:HB3	1:D:201:GLU:CG	2.50	0.41
1:D:2:THR:O	1:D:28:GLU:HB2	2.21	0.41
1:D:68:THR:HG21	1:D:188:MET:HE3	2.02	0.40
1:B:182:PHE:CD1	1:B:188:MET:HE3	2.56	0.40
1:C:23:GLY:HA3	1:C:35:GLU:O	2.21	0.40
1:C:31:ARG:NH1	1:C:206:VAL:HG11	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:106:ASN:N	4:B:1467:HOH:O[2_574]	2.14	0.06

## 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	210/216 (97%)	204 (97%)	6 (3%)	0	100	100
1	B	210/216 (97%)	204 (97%)	6 (3%)	0	100	100
1	C	209/216 (97%)	202 (97%)	6 (3%)	1 (0%)	38	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	210/216 (97%)	203 (97%)	6 (3%)	1 (0%)	38	45
All	All	839/864 (97%)	813 (97%)	24 (3%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	SER
1	D	183	SER

### 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	186/187 (100%)	183 (98%)	3 (2%)	75	88
1	B	186/187 (100%)	186 (100%)	0	100	100
1	C	185/187 (99%)	179 (97%)	6 (3%)	51	67
1	D	186/187 (100%)	181 (97%)	5 (3%)	57	74
All	All	743/748 (99%)	729 (98%)	14 (2%)	69	85

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

Mol	Chain	Res	Type
1	A	14	LEU
1	A	138	ASP
1	A	180	GLU
1	C	132	LYS
1	C	146	ASN
1	C	150	SER
1	C	154	ARG
1	C	180	GLU
1	C	183	SER
1	D	146	ASN
1	D	183	SER
1	D	188	MET
1	D	213	ASN

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Mol	Chain	Res	Type
1	D	218	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	83	ASN
1	A	106	ASN
1	A	122	GLN
1	A	146	ASN
1	B	11	HIS
1	B	83	ASN
1	B	106	ASN
1	B	122	GLN
1	B	146	ASN
1	C	74	HIS
1	C	78	ASN
1	C	83	ASN
1	C	122	GLN
1	C	146	ASN
1	D	74	HIS
1	D	83	ASN
1	D	146	ASN
1	D	213	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are 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	56	1	20,20,21	4.06	7 (35%)	25,27,29	2.46	6 (24%)
1	CR2	B	56	1	20,20,21	4.36	8 (40%)	25,27,29	2.30	7 (28%)
1	CR2	C	56	1	20,20,21	3.98	9 (45%)	25,27,29	2.44	6 (24%)
1	CR2	D	56	1	20,20,21	4.18	8 (40%)	25,27,29	2.37	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	56	1	-	0/8/25/26	0/2/2/2
1	CR2	B	56	1	-	0/8/25/26	0/2/2/2
1	CR2	C	56	1	-	0/8/25/26	0/2/2/2
1	CR2	D	56	1	-	0/8/25/26	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	CR2	O3-C3	16.52	1.22	1.11
1	A	56	CR2	O3-C3	15.52	1.22	1.11
1	D	56	CR2	O3-C3	15.43	1.22	1.11
1	C	56	CR2	O3-C3	14.34	1.21	1.11
1	D	56	CR2	CD2-CG2	4.81	1.48	1.39
1	C	56	CR2	CD2-CG2	4.44	1.48	1.39
1	B	56	CR2	OH-CZ	4.28	1.48	1.37
1	B	56	CR2	CE1-CD1	4.25	1.46	1.38
1	D	56	CR2	OH-CZ	4.22	1.47	1.37
1	D	56	CR2	CE1-CZ	4.20	1.47	1.38
1	C	56	CR2	OH-CZ	4.17	1.47	1.37
1	A	56	CR2	OH-CZ	4.12	1.47	1.37
1	B	56	CR2	CD2-CG2	4.09	1.47	1.39
1	A	56	CR2	CE1-CD1	4.03	1.46	1.38
1	C	56	CR2	CE1-CZ	4.00	1.47	1.38
1	C	56	CR2	CE1-CD1	3.98	1.46	1.38
1	D	56	CR2	CE1-CD1	3.91	1.46	1.38
1	A	56	CR2	CD2-CG2	3.77	1.46	1.39
1	B	56	CR2	CE1-CZ	3.60	1.46	1.38
1	A	56	CR2	CE1-CZ	3.57	1.46	1.38
1	C	56	CR2	C1-N2	3.51	1.40	1.33
1	B	56	CR2	C1-N2	3.37	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	56	CR2	C1-N2	3.11	1.39	1.33
1	B	56	CR2	CD1-CG2	2.96	1.45	1.39
1	D	56	CR2	CD1-CG2	2.87	1.45	1.39
1	A	56	CR2	C1-N2	2.74	1.38	1.33
1	A	56	CR2	CD1-CG2	2.64	1.44	1.39
1	C	56	CR2	CD1-CG2	2.54	1.44	1.39
1	C	56	CR2	CA3-C3	2.40	1.51	1.48
1	C	56	CR2	CE2-CD2	2.20	1.43	1.38
1	B	56	CR2	CE2-CD2	2.07	1.42	1.38
1	D	56	CR2	CE2-CD2	2.01	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	CR2	O2-C2-CA2	-9.11	125.69	130.96
1	A	56	CR2	O2-C2-CA2	-8.91	125.81	130.96
1	D	56	CR2	O2-C2-CA2	-8.32	126.15	130.96
1	B	56	CR2	O2-C2-CA2	-8.12	126.27	130.96
1	A	56	CR2	C1-CA1-N1	-4.69	102.05	112.84
1	C	56	CR2	C1-CA1-N1	-4.69	102.06	112.84
1	B	56	CR2	C1-CA1-N1	-4.48	102.53	112.84
1	D	56	CR2	C1-CA1-N1	-4.46	102.59	112.84
1	A	56	CR2	O2-C2-N3	3.25	131.72	124.71
1	D	56	CR2	O2-C2-N3	3.20	131.61	124.71
1	D	56	CR2	N3-C1-N2	-3.18	108.72	111.56
1	C	56	CR2	O2-C2-N3	3.15	131.50	124.71
1	B	56	CR2	N3-C1-N2	-3.13	108.77	111.56
1	A	56	CR2	N3-C1-N2	-3.12	108.78	111.56
1	C	56	CR2	N3-C1-N2	-2.99	108.89	111.56
1	B	56	CR2	O2-C2-N3	2.98	131.12	124.71
1	D	56	CR2	C2-N3-C1	2.40	114.00	108.63
1	B	56	CR2	C2-N3-C1	2.39	113.97	108.63
1	A	56	CR2	C2-N3-C1	2.25	113.68	108.63
1	A	56	CR2	CE1-CD1-CG2	-2.21	118.52	121.30
1	C	56	CR2	CE1-CD1-CG2	-2.16	118.58	121.30
1	D	56	CR2	CA2-C2-N3	-2.14	102.22	103.44
1	C	56	CR2	C2-N3-C1	2.13	113.39	108.63
1	B	56	CR2	CA1-C1-N2	2.12	126.33	123.82
1	B	56	CR2	CE1-CD1-CG2	-2.09	118.66	121.30
1	D	56	CR2	CE1-CD1-CG2	-2.09	118.67	121.30
1	D	56	CR2	CA1-C1-N2	2.08	126.29	123.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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$
2	CXS	A	1003	-	14,14,14	1.19	2 (14%)	18,18,18	2.08	8 (44%)
2	CXS	B	1001	-	14,14,14	1.07	1 (7%)	18,18,18	2.15	8 (44%)
2	CXS	B	1002	-	14,14,14	1.25	2 (14%)	18,18,18	2.01	8 (44%)
2	CXS	B	1004	-	14,14,14	1.20	2 (14%)	18,18,18	2.10	8 (44%)
2	CXS	D	1005	-	14,14,14	1.26	2 (14%)	18,18,18	2.01	8 (44%)

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
2	CXS	A	1003	-	-	0/8/16/16	0/1/1/1
2	CXS	B	1001	-	-	0/8/16/16	0/1/1/1
2	CXS	B	1002	-	-	0/8/16/16	0/1/1/1
2	CXS	B	1004	-	-	0/8/16/16	0/1/1/1
2	CXS	D	1005	-	-	0/8/16/16	0/1/1/1

All (9) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1005	CXS	C1-S	2.95	1.82	1.77
2	A	1003	CXS	C1-S	2.91	1.81	1.77
2	B	1002	CXS	C1-S	2.90	1.81	1.77
2	B	1004	CXS	C1-S	2.64	1.81	1.77
2	B	1001	CXS	O3-S	2.48	1.52	1.46
2	B	1002	CXS	O3-S	2.33	1.52	1.46
2	B	1004	CXS	O3-S	2.28	1.51	1.46
2	A	1003	CXS	O3-S	2.12	1.51	1.46
2	D	1005	CXS	O3-S	2.03	1.51	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1005	CXS	O2-S-C1	4.22	110.43	106.81
2	B	1002	CXS	O2-S-C1	4.00	110.24	106.81
2	A	1003	CXS	O2-S-C1	3.87	110.13	106.81
2	B	1004	CXS	C2-C1-S	-3.82	108.31	113.24
2	B	1004	CXS	C3-N-C4	-3.61	106.35	113.98
2	B	1001	CXS	O2-S-C1	3.54	109.84	106.81
2	A	1003	CXS	C3-N-C4	-3.42	106.75	113.98
2	B	1001	CXS	O3-S-C1	-3.40	101.62	105.93
2	B	1001	CXS	O1-S-C1	3.39	109.71	106.81
2	B	1004	CXS	O2-S-C1	3.36	109.69	106.81
2	B	1001	CXS	C3-N-C4	-3.23	107.15	113.98
2	B	1001	CXS	C2-C1-S	-3.22	109.09	113.24
2	B	1001	CXS	O3-S-O1	-3.08	105.12	111.78
2	B	1002	CXS	O3-S-O1	-3.06	105.16	111.78
2	A	1003	CXS	O3-S-C1	-3.04	102.08	105.93
2	A	1003	CXS	C2-C1-S	-3.02	109.34	113.24
2	B	1002	CXS	O3-S-C1	-3.01	102.11	105.93
2	D	1005	CXS	O3-S-C1	-3.01	102.12	105.93
2	B	1004	CXS	O1-S-C1	2.94	109.33	106.81
2	D	1005	CXS	C2-C1-S	-2.89	109.52	113.24
2	D	1005	CXS	O3-S-O1	-2.86	105.59	111.78
2	B	1004	CXS	O3-S-O1	-2.81	105.70	111.78
2	B	1004	CXS	O3-S-C1	-2.78	102.40	105.93
2	A	1003	CXS	O1-S-C1	2.78	109.19	106.81
2	B	1002	CXS	O1-S-C1	2.74	109.16	106.81
2	A	1003	CXS	O3-S-O1	-2.74	105.85	111.78
2	D	1005	CXS	O1-S-C1	2.72	109.14	106.81
2	B	1002	CXS	C2-C1-S	-2.70	109.75	113.24
2	A	1003	CXS	O3-S-O2	-2.64	106.08	111.78
2	B	1004	CXS	O3-S-O2	-2.47	106.45	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1005	CXS	O3-S-O2	-2.39	106.62	111.78
2	A	1003	CXS	O2-S-O1	2.34	121.60	113.26
2	B	1004	CXS	O2-S-O1	2.30	121.47	113.26
2	B	1002	CXS	O2-S-O1	2.29	121.42	113.26
2	B	1002	CXS	O3-S-O2	-2.28	106.86	111.78
2	B	1002	CXS	C3-N-C4	-2.27	109.18	113.98
2	B	1001	CXS	O2-S-O1	2.27	121.36	113.26
2	D	1005	CXS	C3-N-C4	-2.26	109.21	113.98
2	D	1005	CXS	O2-S-O1	2.20	121.11	113.26
2	B	1001	CXS	O3-S-O2	-2.10	107.24	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	215/216 (99%)	-0.38	3 (1%) 72 80	9, 18, 37, 66	0
1	B	215/216 (99%)	-0.37	4 (1%) 64 73	8, 18, 40, 70	0
1	C	214/216 (99%)	-0.14	11 (5%) 27 37	10, 21, 46, 65	0
1	D	215/216 (99%)	-0.09	13 (6%) 21 30	9, 22, 48, 79	0
All	All	859/864 (99%)	-0.24	31 (3%) 41 51	8, 20, 44, 79	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	ASP	9.4
1	B	218	ASP	6.9
1	A	218	ASP	5.6
1	B	2	THR	4.9
1	D	185	SER	4.3
1	D	2	THR	3.9
1	D	40	ASP	3.9
1	C	180	GLU	3.6
1	D	180	GLU	3.6
1	C	2	THR	3.4
1	B	180	GLU	3.4
1	C	145	GLY	3.3
1	C	185	SER	3.2
1	D	145	GLY	3.2
1	C	183	SER	3.2
1	D	216	PRO	3.1
1	C	66	LYS	3.1
1	D	78	ASN	3.0
1	C	40	ASP	3.0
1	D	183	SER	2.9
1	C	78	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	2.7
1	A	180	GLU	2.5
1	D	3	THR	2.4
1	C	216	PRO	2.3
1	C	217	ARG	2.2
1	B	78	ASN	2.2
1	C	146	ASN	2.1
1	D	66	LYS	2.1
1	D	67	GLY	2.0
1	D	175	LYS	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	56	19/20	0.13	0.84	9,11,16,17	0
1	CR2	B	56	19/20	0.13	0.53	9,12,17,18	0
1	CR2	C	56	19/20	0.14	0.49	12,15,17,18	0
1	CR2	D	56	19/20	0.12	-0.09	10,14,16,17	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
2	CXS	B	1001	14/14	0.28	3.03	51,54,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CXS	B	1002	14/14	0.13	2.50	18,22,34,38	0
2	CXS	D	1005	14/14	0.11	1.90	18,22,33,36	0
2	CXS	B	1004	14/14	0.15	1.17	49,54,56,56	0
2	CXS	A	1003	14/14	0.14	0.72	49,53,54,55	0
3	CL	B	1006	1/1	0.03	-3.92	13,13,13,13	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.