



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:16 am GMT

PDB ID : 1G7K  
Title : CRYSTAL STRUCTURE OF DSRED, A RED FLUORESCENT PROTEIN FROM DISCOSOMA SP. RED  
Authors : Yarbrough, D.; Wachter, R.M.; Kallio, K.; Matz, M.V.; Remington, S.J.  
Deposited on : 2000-11-10  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

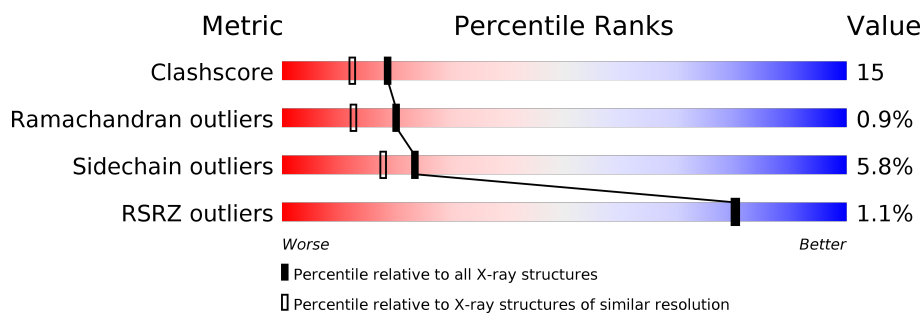
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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. 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	234	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>5%</div> <div>7%</div> </div> </div>
1	B	234	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	234	<div> <div></div> <div> <div>60%</div> <div>26%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	234	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>29%</div> <div>• •</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7586 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 FLUORESCENT PROTEIN FP583.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	B	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	C	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			
1	D	218	Total	C	N	O	S	Se	0	1	0
			1792	1159	298	328	1	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	INSERTION	UNP Q9U6Y8
A	-9	ARG	-	INSERTION	UNP Q9U6Y8
A	-8	GLY	-	INSERTION	UNP Q9U6Y8
A	-7	SER	-	INSERTION	UNP Q9U6Y8
A	-6	HIS	-	INSERTION	UNP Q9U6Y8
A	-5	HIS	-	INSERTION	UNP Q9U6Y8
A	-4	HIS	-	INSERTION	UNP Q9U6Y8
A	-3	HIS	-	INSERTION	UNP Q9U6Y8
A	-2	HIS	-	INSERTION	UNP Q9U6Y8
A	-1	HIS	-	INSERTION	UNP Q9U6Y8
A	0	GLY	-	INSERTION	UNP Q9U6Y8
A	1	SER	-	INSERTION	UNP Q9U6Y8
A	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
A	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
B	-10	MSE	-	INSERTION	UNP Q9U6Y8
B	-9	ARG	-	INSERTION	UNP Q9U6Y8
B	-8	GLY	-	INSERTION	UNP Q9U6Y8
B	-7	SER	-	INSERTION	UNP Q9U6Y8
B	-6	HIS	-	INSERTION	UNP Q9U6Y8
B	-5	HIS	-	INSERTION	UNP Q9U6Y8

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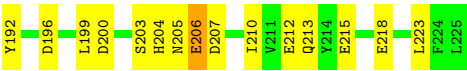
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	INSERTION	UNP Q9U6Y8
B	-3	HIS	-	INSERTION	UNP Q9U6Y8
B	-2	HIS	-	INSERTION	UNP Q9U6Y8
B	-1	HIS	-	INSERTION	UNP Q9U6Y8
B	0	GLY	-	INSERTION	UNP Q9U6Y8
B	1	SER	-	INSERTION	UNP Q9U6Y8
B	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
B	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
C	-10	MSE	-	INSERTION	UNP Q9U6Y8
C	-9	ARG	-	INSERTION	UNP Q9U6Y8
C	-8	GLY	-	INSERTION	UNP Q9U6Y8
C	-7	SER	-	INSERTION	UNP Q9U6Y8
C	-6	HIS	-	INSERTION	UNP Q9U6Y8
C	-5	HIS	-	INSERTION	UNP Q9U6Y8
C	-4	HIS	-	INSERTION	UNP Q9U6Y8
C	-3	HIS	-	INSERTION	UNP Q9U6Y8
C	-2	HIS	-	INSERTION	UNP Q9U6Y8
C	-1	HIS	-	INSERTION	UNP Q9U6Y8
C	0	GLY	-	INSERTION	UNP Q9U6Y8
C	1	SER	-	INSERTION	UNP Q9U6Y8
C	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
C	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8
D	-10	MSE	-	INSERTION	UNP Q9U6Y8
D	-9	ARG	-	INSERTION	UNP Q9U6Y8
D	-8	GLY	-	INSERTION	UNP Q9U6Y8
D	-7	SER	-	INSERTION	UNP Q9U6Y8
D	-6	HIS	-	INSERTION	UNP Q9U6Y8
D	-5	HIS	-	INSERTION	UNP Q9U6Y8
D	-4	HIS	-	INSERTION	UNP Q9U6Y8
D	-3	HIS	-	INSERTION	UNP Q9U6Y8
D	-2	HIS	-	INSERTION	UNP Q9U6Y8
D	-1	HIS	-	INSERTION	UNP Q9U6Y8
D	0	GLY	-	INSERTION	UNP Q9U6Y8
D	1	SER	-	INSERTION	UNP Q9U6Y8
D	66	CRQ	GLN	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	TYR	CHROMOPHORE	UNP Q9U6Y8
D	66	CRQ	GLY	CHROMOPHORE	UNP Q9U6Y8

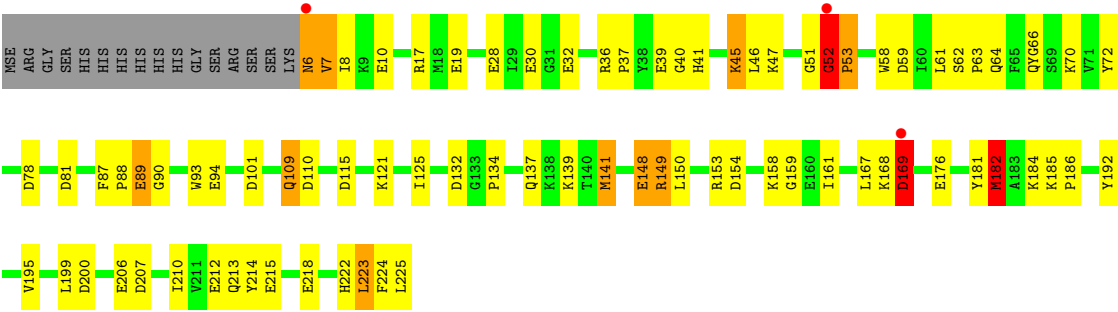
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total 96	O 96	0	0
2	B	116	Total 116	O 116	0	0
2	C	100	Total 100	O 100	0	0
2	D	106	Total 106	O 106	0	0





● Molecule 1: FLUORESCENT PROTEIN FP583



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.37Å 112.27Å 70.69Å 90.00° 93.81° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 25.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.00) 95.2 (25.14-2.00)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	36.12 (at 1.99Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.162 , 0.249 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	8.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: CRQ

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	1.14	13/1815 (0.7%)	1.32	25/2435 (1.0%)
1	B	1.11	12/1815 (0.7%)	1.30	26/2435 (1.1%)
1	C	1.10	12/1815 (0.7%)	1.12	16/2435 (0.7%)
1	D	1.08	12/1815 (0.7%)	1.30	24/2435 (1.0%)
All	All	1.11	49/7260 (0.7%)	1.26	91/9740 (0.9%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CD-OE2	8.93	1.35	1.25
1	C	94	GLU	CD-OE2	8.19	1.34	1.25
1	C	218	GLU	CD-OE2	7.91	1.34	1.25
1	D	148	GLU	CD-OE2	7.14	1.33	1.25
1	C	32	GLU	CD-OE2	7.04	1.33	1.25
1	B	94	GLU	CD-OE2	6.97	1.33	1.25
1	B	206	GLU	CD-OE2	6.87	1.33	1.25
1	B	160	GLU	CD-OE2	6.85	1.33	1.25
1	D	218	GLU	CD-OE2	6.76	1.33	1.25
1	B	30	GLU	CD-OE2	6.66	1.32	1.25
1	A	176	GLU	CD-OE2	6.64	1.32	1.25
1	A	218	GLU	CD-OE2	6.59	1.32	1.25
1	A	39	GLU	CD-OE2	6.48	1.32	1.25
1	B	89	GLU	CD-OE2	6.43	1.32	1.25
1	A	30	GLU	CD-OE2	6.35	1.32	1.25
1	D	94	GLU	CD-OE2	6.35	1.32	1.25
1	C	39	GLU	CD-OE2	6.34	1.32	1.25
1	B	32	GLU	CD-OE2	6.33	1.32	1.25
1	C	144	GLU	CD-OE1	-6.33	1.18	1.25
1	A	94	GLU	CD-OE2	6.20	1.32	1.25
1	C	100	GLU	CD-OE2	6.14	1.32	1.25
1	D	28	GLU	CD-OE2	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	34	GLU	CD-OE2	6.04	1.32	1.25
1	B	10	GLU	CD-OE2	6.04	1.32	1.25
1	C	212	GLU	CD-OE2	6.04	1.32	1.25
1	D	30	GLU	CD-OE2	5.96	1.32	1.25
1	D	32	GLU	CD-OE2	5.88	1.32	1.25
1	B	218	GLU	CD-OE2	5.79	1.32	1.25
1	C	30	GLU	CD-OE2	5.78	1.32	1.25
1	D	176	GLU	CD-OE2	5.76	1.31	1.25
1	D	215	GLU	CD-OE2	5.73	1.31	1.25
1	A	215	GLU	CD-OE2	5.70	1.31	1.25
1	A	19	GLU	CD-OE2	5.68	1.31	1.25
1	D	39	GLU	CD-OE2	5.68	1.31	1.25
1	D	19	GLU	CD-OE2	5.63	1.31	1.25
1	A	34	GLU	CD-OE2	5.63	1.31	1.25
1	C	10	GLU	CD-OE2	5.60	1.31	1.25
1	B	148	GLU	CD-OE2	5.55	1.31	1.25
1	B	26	GLU	CD-OE2	5.50	1.31	1.25
1	A	10	GLU	CD-OE2	5.48	1.31	1.25
1	D	89	GLU	CD-OE2	5.44	1.31	1.25
1	D	206	GLU	CD-OE2	5.44	1.31	1.25
1	C	206	GLU	CD-OE1	-5.38	1.19	1.25
1	A	160	GLU	CD-OE2	5.34	1.31	1.25
1	B	215	GLU	CD-OE2	5.32	1.31	1.25
1	A	32	GLU	CD-OE2	5.30	1.31	1.25
1	C	215	GLU	CD-OE2	5.22	1.31	1.25
1	B	94	GLU	CD-OE1	-5.17	1.20	1.25
1	A	89	GLU	CD-OE2	5.13	1.31	1.25

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLY	C-N-CD	-30.86	52.72	120.60
1	D	52	GLY	C-N-CD	-30.34	53.85	120.60
1	B	52	GLY	C-N-CD	-28.26	58.44	120.60
1	A	53	PRO	N-CA-CB	8.88	113.96	103.30
1	B	36	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	53	PRO	N-CA-CB	7.98	112.88	103.30
1	D	153	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	196	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	59	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	59	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	196	ASP	CB-CG-OD2	-6.67	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	CB-CG-OD1	6.66	124.29	118.30
1	D	81	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	59	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	D	200	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	D	207	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	52	GLY	O-C-N	6.30	133.07	121.10
1	C	196	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	132	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	81	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	C	132	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	B	52	GLY	O-C-N	6.14	132.77	121.10
1	B	196	ASP	CB-CG-OD1	6.13	123.82	118.30
1	D	78	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	81	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	182	MSE	CG-SE-CE	-6.02	85.67	98.90
1	A	132	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	169	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	115	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	207	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	101	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	59	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	196	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	101	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	D	132	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	182	MSE	CG-SE-CE	-5.81	86.12	98.90
1	A	132	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	200	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	132	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	59	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	81	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	154	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	207	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	D	169	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	115	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	200	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	101	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	154	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	59	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	95	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	132	ASP	CB-CG-OD1	5.54	123.28	118.30
1	D	182	MSE	CG-SE-CE	-5.53	86.73	98.90
1	D	101	ASP	CB-CG-OD1	5.51	123.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	59	ASP	CB-CG-OD1	5.45	123.20	118.30
1	C	95	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	101	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	169	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	207	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	154	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	52	GLY	C-N-CA	5.41	144.71	122.00
1	B	59	ASP	CB-CG-OD1	5.39	123.16	118.30
1	B	78	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	78	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	D	200	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	200	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	C	110	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	154	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	95	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	110	ASP	CB-CG-OD1	5.30	123.08	118.30
1	B	115	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	149	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	169	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	132	ASP	CB-CG-OD1	5.28	123.05	118.30
1	C	110	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	154	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	110	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	115	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	115	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	110	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	52	GLY	C-N-CA	5.15	143.62	122.00
1	A	110	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	81	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	154	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	81	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	36	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	D	115	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	110	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	53	PRO	CA-N-CD	-5.03	104.46	111.50
1	A	207	ASP	CB-CG-OD1	5.00	122.80	118.30
1	C	101	ASP	CB-CG-OD1	5.00	122.80	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	A	1792	0	1746	48	0
1	B	1792	0	1746	60	0
1	C	1792	0	1746	48	0
1	D	1792	0	1746	61	0
2	A	96	0	0	6	0
2	B	116	0	0	6	0
2	C	100	0	0	1	0
2	D	106	0	0	2	0
All	All	7586	0	6984	209	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 15.

All (209) 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:6:ASN:HA	1:C:7:VAL:HB	1.42	1.00
1:B:141:MSE:HE3	1:B:168:LYS:HG2	1.46	0.95
1:D:141:MSE:HE3	1:D:168:LYS:HG2	1.50	0.94
1:D:148:GLU:HB3	1:D:195:VAL:HG23	1.51	0.92
1:B:17:ARG:HH12	1:B:19:GLU:HG3	1.35	0.92
1:D:150:LEU:HD11	1:D:195:VAL:HG22	1.52	0.91
1:B:45:LYS:HE2	1:B:47:LYS:HZ1	1.33	0.90
1:B:45:LYS:HE2	1:B:47:LYS:NZ	1.87	0.88
1:C:45:LYS:HE2	1:C:47:LYS:HE3	1.60	0.83
1:B:132:ASP:HA	1:B:137:GLN:HE21	1.45	0.81
1:C:134:PRO:HA	1:C:139:LYS:HG2	1.62	0.81
1:B:17:ARG:NH1	1:B:19:GLU:HG3	1.96	0.80
1:A:158:LYS:HE2	1:A:180:ILE:HD12	1.64	0.80
1:B:45:LYS:HE2	1:B:47:LYS:CE	2.11	0.80
1:A:45:LYS:CD	1:A:212:GLU:HG3	2.12	0.79
1:C:36:ARG:HG3	1:C:41:HIS:CE1	2.20	0.77
1:C:82:TYR:CD1	1:C:187:VAL:HG22	2.20	0.77
1:B:45:LYS:HE2	1:B:47:LYS:HE3	1.66	0.76
1:D:134:PRO:HA	1:D:139:LYS:HE3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LEU:HD11	1:D:195:VAL:CG2	2.20	0.72
1:D:150:LEU:CD1	1:D:195:VAL:HG22	2.19	0.72
1:A:16:VAL:C	1:A:17:ARG:HD2	2.10	0.71
1:B:9:LYS:HE3	2:B:294:HOH:O	1.90	0.71
1:C:45:LYS:CE	1:C:47:LYS:HE3	2.20	0.71
1:A:6:ASN:ND2	1:A:9:LYS:HG3	2.06	0.71
1:B:58:TRP:HE1	1:B:213:GLN:HE21	1.39	0.70
1:D:148:GLU:HB3	1:D:195:VAL:CG2	2.21	0.70
1:A:16:VAL:N	1:A:17:ARG:HH11	1.89	0.70
1:B:181:TYR:C	1:B:182:MSE:HG3	2.11	0.70
1:D:137:GLN:HB2	1:D:139:LYS:HE2	1.72	0.70
1:D:109:GLN:HB2	1:D:121:LYS:O	1.91	0.70
1:A:45:LYS:HD3	1:A:212:GLU:HG3	1.73	0.69
1:D:47:LYS:HD3	1:D:210:ILE:HG12	1.76	0.67
1:B:17:ARG:HD3	2:B:313:HOH:O	1.95	0.67
1:B:132:ASP:HA	1:B:137:GLN:NE2	2.10	0.66
1:A:181:TYR:C	1:A:182:MSE:HG3	2.14	0.66
1:B:17:ARG:HG2	1:B:17:ARG:HH11	1.58	0.66
1:B:216:ARG:HG2	1:D:224:PHE:CE2	2.31	0.66
1:C:181:TYR:C	1:C:182:MSE:HG3	2.14	0.66
1:C:134:PRO:HB3	1:C:139:LYS:HG3	1.78	0.66
1:A:16:VAL:N	1:A:17:ARG:NH1	2.44	0.65
1:A:6:ASN:HD21	1:A:9:LYS:HG3	1.62	0.65
1:B:76:PRO:HG2	1:B:79:ILE:HD12	1.79	0.65
1:D:89:GLU:OE1	1:D:185:LYS:HD3	1.95	0.65
1:D:222:HIS:HB3	1:D:225:LEU:HG	1.78	0.65
1:C:17:ARG:NH1	1:C:30:GLU:OE1	2.30	0.64
1:D:149:ARG:HD3	1:D:192:TYR:CZ	2.32	0.64
1:A:6:ASN:O	1:A:7:VAL:HG13	1.97	0.64
1:D:141:MSE:HE3	1:D:168:LYS:CG	2.28	0.64
1:B:17:ARG:HH12	1:B:19:GLU:CG	2.10	0.63
1:C:36:ARG:HG3	1:C:41:HIS:HE1	1.64	0.63
1:B:216:ARG:HD2	1:B:218:GLU:OE2	1.99	0.62
1:C:106:THR:HG23	1:D:125:ILE:CG2	2.29	0.62
1:D:40:GLY:HA2	1:D:72:TYR:O	1.99	0.62
1:B:141:MSE:HE3	1:B:168:LYS:CG	2.26	0.62
1:B:144:GLU:OE2	1:B:172:HIS:HE1	1.83	0.62
1:B:58:TRP:HE1	1:B:213:GLN:NE2	1.97	0.62
1:A:16:VAL:H	1:A:17:ARG:NH1	1.97	0.62
1:A:58:TRP:HE1	1:A:213:GLN:HE21	1.48	0.61
1:A:52:GLY:HA3	2:A:288:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:TYR:C	1:D:182:MSE:HG3	2.18	0.61
1:D:148:GLU:OE1	1:D:195:VAL:HG21	1.99	0.61
1:D:87:PHE:HB3	1:D:88:PRO:HA	1.83	0.60
1:C:94:GLU:HG3	1:C:180:ILE:HD13	1.83	0.60
1:A:134:PRO:HA	1:A:139:LYS:HD2	1.84	0.60
1:B:141:MSE:CE	1:B:168:LYS:HG2	2.28	0.60
1:C:134:PRO:HA	1:C:139:LYS:CG	2.31	0.60
1:A:17:ARG:HG3	1:A:30:GLU:HG2	1.84	0.60
1:A:58:TRP:HE1	1:A:213:GLN:NE2	2.00	0.59
1:D:141:MSE:SE	1:D:168:LYS:HA	2.52	0.59
1:A:45:LYS:HD2	1:A:212:GLU:HG3	1.83	0.59
1:C:62:SER:OG	1:C:63:PRO:HD3	2.01	0.59
1:B:79:ILE:HG12	2:B:331:HOH:O	2.03	0.58
1:B:47:LYS:HG3	1:B:210:ILE:HG12	1.85	0.58
1:D:141:MSE:CE	1:D:168:LYS:HG2	2.30	0.58
1:B:75:HIS:HE1	1:B:193:TYR:OH	1.85	0.58
1:B:123:LYS:NZ	2:B:313:HOH:O	2.28	0.57
1:C:58:TRP:HE1	1:C:213:GLN:NE2	2.02	0.57
1:C:89:GLU:OE1	1:C:185:LYS:NZ	2.29	0.57
1:B:149:ARG:HD3	1:B:192:TYR:CZ	2.39	0.57
1:B:172:HIS:HD2	2:D:281:HOH:O	1.88	0.57
1:C:58:TRP:HE1	1:C:213:GLN:HE21	1.52	0.56
1:B:66:CRQ:HE1	1:B:199:LEU:HB2	1.88	0.56
1:D:66:CRQ:HE1	1:D:199:LEU:HB2	1.88	0.56
1:A:158:LYS:HE2	1:A:180:ILE:CD1	2.32	0.56
1:A:114:GLN:HG3	1:A:119:ILE:HG13	1.88	0.55
1:D:6:ASN:O	1:D:7:VAL:HG22	2.07	0.54
1:A:149:ARG:HD3	1:A:192:TYR:CZ	2.43	0.54
1:B:216:ARG:HG3	1:B:217:THR:N	2.21	0.54
1:C:92:LYS:NZ	1:C:110:ASP:OD1	2.40	0.54
1:C:17:ARG:HG2	1:C:30:GLU:HG2	1.90	0.54
1:D:45:LYS:HD3	1:D:212:GLU:OE1	2.08	0.54
1:A:47:LYS:HG2	1:A:210:ILE:HG12	1.90	0.53
1:C:149:ARG:HD3	1:C:192:TYR:CZ	2.43	0.53
1:A:43:THR:HG22	1:A:214:TYR:HD1	1.73	0.53
1:B:119:ILE:HG21	1:B:121:LYS:HZ1	1.73	0.53
1:D:70:LYS:HE2	2:D:270:HOH:O	2.08	0.53
1:C:40:GLY:HA2	1:C:72:TYR:O	2.07	0.53
1:B:18:MSE:HE3	1:B:65:PHE:CE2	2.43	0.53
1:D:62:SER:OG	1:D:63:PRO:HD3	2.09	0.53
1:B:6:ASN:ND2	1:B:8:ILE:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LYS:CE	1:B:47:LYS:HE3	2.37	0.52
1:A:28:GLU:HB2	1:A:50:LYS:HG3	1.92	0.52
1:A:180:ILE:HD11	1:B:128:ASN:OD1	2.10	0.52
1:D:45:LYS:HB2	1:D:212:GLU:HG2	1.92	0.52
1:B:122:VAL:C	1:B:123:LYS:HD2	2.31	0.51
1:A:16:VAL:O	1:A:17:ARG:NH1	2.44	0.51
1:D:134:PRO:CA	1:D:139:LYS:HE3	2.40	0.51
1:C:6:ASN:CA	1:C:7:VAL:HB	2.29	0.51
1:C:199:LEU:C	1:C:199:LEU:HD23	2.31	0.51
1:D:93:TRP:CE2	1:D:109:GLN:HG3	2.46	0.50
1:D:149:ARG:HD3	1:D:192:TYR:CE1	2.46	0.50
1:A:178:LYS:NZ	2:A:265:HOH:O	2.43	0.50
1:A:128:ASN:OD1	1:B:158:LYS:NZ	2.44	0.50
1:B:90:GLY:C	1:B:184:LYS:HD2	2.32	0.50
1:B:70:LYS:HD2	1:B:73:VAL:CG2	2.42	0.50
1:B:141:MSE:HE3	1:B:168:LYS:HA	1.93	0.50
1:A:14:PHE:HB3	1:A:118:PHE:HB2	1.93	0.49
1:D:51:GLY:O	1:D:52:GLY:O	2.29	0.49
1:C:70:LYS:HE2	2:C:269:HOH:O	2.12	0.49
1:D:6:ASN:C	1:D:8:ILE:H	2.14	0.49
1:B:17:ARG:HH11	1:B:17:ARG:CG	2.22	0.49
1:D:52:GLY:O	1:D:53:PRO:O	2.29	0.49
1:B:121:LYS:HE2	2:B:227:HOH:O	2.12	0.49
1:C:6:ASN:OD1	1:C:8:ILE:O	2.30	0.49
1:C:167:LEU:HD11	1:C:173:TYR:HB2	1.95	0.49
1:D:148:GLU:HG2	1:D:150:LEU:CD1	2.44	0.48
1:C:6:ASN:OD1	1:C:8:ILE:HB	2.14	0.48
1:D:148:GLU:HB2	1:D:161:ILE:HG12	1.94	0.48
1:D:45:LYS:HD3	1:D:212:GLU:CD	2.34	0.48
1:A:6:ASN:HD21	1:A:9:LYS:CG	2.25	0.48
1:A:54:LEU:O	1:A:138:LYS:NZ	2.31	0.48
1:C:36:ARG:HB2	1:C:39:GLU:HB2	1.96	0.48
1:D:93:TRP:CE2	1:D:109:GLN:CG	2.97	0.47
1:D:89:GLU:H	1:D:89:GLU:CD	2.17	0.47
1:C:89:GLU:CD	1:C:89:GLU:H	2.17	0.47
1:A:17:ARG:NH1	1:A:31:GLY:O	2.40	0.47
1:C:106:THR:HG23	1:D:125:ILE:HG21	1.96	0.47
1:C:204:HIS:HD2	1:C:205:ASN:O	1.97	0.47
1:D:223:LEU:HD12	1:D:223:LEU:HA	1.73	0.47
1:D:62:SER:HA	1:D:213:GLN:HE22	1.80	0.47
1:B:119:ILE:HG21	1:B:121:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LYS:O	1:C:168:LYS:NZ	2.48	0.46
1:D:45:LYS:HB2	1:D:212:GLU:CG	2.45	0.46
1:A:41:HIS:HD2	2:A:242:HOH:O	1.97	0.46
1:B:91:PHE:N	1:B:184:LYS:HD2	2.31	0.46
1:D:46:LEU:HD22	1:D:46:LEU:N	2.29	0.46
1:A:16:VAL:C	1:A:17:ARG:HH11	2.19	0.46
1:D:37:PRO:HA	1:D:72:TYR:HA	1.98	0.46
1:A:149:ARG:HD2	1:A:149:ARG:C	2.35	0.46
1:C:106:THR:CG2	1:D:125:ILE:HB	2.45	0.46
1:A:137:GLN:HB2	1:A:139:LYS:HD2	1.98	0.46
1:A:52:GLY:HA3	2:A:263:HOH:O	2.16	0.45
1:A:153:ARG:CG	1:A:154:ASP:N	2.79	0.45
1:C:59:ASP:HB3	1:C:165:LEU:HD21	1.98	0.45
1:D:93:TRP:NE1	1:D:109:GLN:CG	2.79	0.45
1:B:149:ARG:HD3	1:B:192:TYR:CE1	2.50	0.45
1:B:62:SER:OG	1:B:63:PRO:HD3	2.16	0.45
1:B:196:ASP:O	1:B:217:THR:HA	2.16	0.45
1:A:105:VAL:HG22	1:A:126:GLY:HA2	1.98	0.45
1:D:169:ASP:N	1:D:169:ASP:OD2	2.44	0.45
1:C:66:CRQ:HE1	1:C:199:LEU:HB2	1.98	0.44
1:D:137:GLN:CB	1:D:139:LYS:HE2	2.44	0.44
1:A:17:ARG:HD2	1:A:17:ARG:N	2.32	0.44
1:B:17:ARG:NH1	1:B:17:ARG:CG	2.79	0.44
1:B:199:LEU:HD23	1:B:199:LEU:C	2.37	0.44
1:C:134:PRO:HA	1:C:139:LYS:HE2	1.99	0.44
1:B:94:GLU:HG2	1:B:108:THR:HA	2.00	0.44
1:A:121:LYS:NZ	2:A:276:HOH:O	2.29	0.44
1:A:36:ARG:NE	1:A:39:GLU:OE1	2.45	0.44
1:A:134:PRO:HA	1:A:139:LYS:CD	2.46	0.44
1:A:94:GLU:HG2	1:A:108:THR:HA	2.00	0.44
1:B:71:VAL:HG12	2:B:255:HOH:O	2.18	0.44
1:D:90:GLY:C	1:D:184:LYS:HD2	2.38	0.44
1:D:66:CRQ:NE1	1:D:213:GLN:OE1	2.50	0.44
1:B:62:SER:HA	1:B:213:GLN:HE22	1.83	0.43
1:D:10:GLU:O	1:D:36:ARG:HD2	2.18	0.43
1:D:58:TRP:HE1	1:D:213:GLN:HE21	1.66	0.43
1:C:25:HIS:HE1	1:C:51:GLY:O	2.01	0.43
1:D:41:HIS:ND1	1:D:214:TYR:OH	2.39	0.43
1:B:6:ASN:HD21	1:B:8:ILE:HB	1.83	0.43
1:D:149:ARG:O	1:D:159:GLY:HA2	2.19	0.42
1:D:141:MSE:HB3	1:D:141:MSE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLN:N	1:B:119:ILE:CD1	2.82	0.42
1:D:45:LYS:HD3	1:D:212:GLU:CG	2.49	0.42
1:A:36:ARG:HE	1:A:39:GLU:CD	2.23	0.42
1:B:19:GLU:HB2	1:B:123:LYS:HE3	2.01	0.42
1:B:87:PHE:HB3	1:B:88:PRO:HA	2.01	0.42
1:A:71:VAL:O	1:A:71:VAL:HG22	2.20	0.42
1:B:71:VAL:O	1:B:71:VAL:HG22	2.19	0.42
1:D:61:LEU:O	1:D:64:GLN:HG2	2.19	0.42
1:C:106:THR:CG2	1:D:125:ILE:CG2	2.98	0.42
1:A:62:SER:OG	1:A:63:PRO:HD3	2.20	0.41
1:A:114:GLN:CG	1:A:119:ILE:HG13	2.49	0.41
1:C:167:LEU:HD12	1:C:167:LEU:HA	1.76	0.41
1:D:199:LEU:HD23	1:D:199:LEU:C	2.41	0.41
1:C:47:LYS:HG3	1:C:210:ILE:HG12	2.02	0.41
1:C:166:LYS:HB2	1:C:166:LYS:HE3	1.89	0.41
1:A:70:LYS:HE3	2:A:237:HOH:O	2.20	0.41
1:C:141:MSE:SE	1:C:168:LYS:HG3	2.71	0.41
1:C:128:ASN:OD1	1:D:158:LYS:NZ	2.50	0.41
1:C:76:PRO:HG2	1:C:79:ILE:HD12	2.02	0.41
1:B:46:LEU:O	1:B:47:LYS:HD2	2.21	0.40
1:C:143:TRP:CZ3	1:C:165:LEU:HG	2.56	0.40
1:C:17:ARG:CG	1:C:30:GLU:HG2	2.51	0.40
1:B:157:LEU:C	1:B:158:LYS:HG2	2.40	0.40
1:B:47:LYS:HE3	1:B:210:ILE:HG23	2.03	0.40
1:C:52:GLY:HA2	1:C:53:PRO:C	2.42	0.40
1:C:99:PHE:HD2	1:C:173:TYR:CE2	2.39	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	216/234 (92%)	209 (97%)	5 (2%)	2 (1%)	20	12
1	B	216/234 (92%)	209 (97%)	6 (3%)	1 (0%)	32	26
1	C	216/234 (92%)	209 (97%)	6 (3%)	1 (0%)	32	26
1	D	216/234 (92%)	206 (95%)	6 (3%)	4 (2%)	9	4
All	All	864/936 (92%)	833 (96%)	23 (3%)	8 (1%)	20	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	53	PRO
1	B	53	PRO
1	C	7	VAL
1	D	52	GLY
1	D	53	PRO
1	D	7	VAL
1	D	186	PRO

### 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	192/198 (97%)	184 (96%)	8 (4%)	34	30
1	B	192/198 (97%)	181 (94%)	11 (6%)	24	18
1	C	192/198 (97%)	175 (91%)	17 (9%)	11	7
1	D	192/198 (97%)	183 (95%)	9 (5%)	30	26
All	All	768/792 (97%)	723 (94%)	45 (6%)	23	17

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	9	LYS
1	A	121	LYS

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Mol	Chain	Res	Type
1	A	134	PRO
1	A	167	LEU
1	A	182	MSE
1	A	203	SER
1	A	223	LEU
1	B	9	LYS
1	B	10	GLU
1	B	32	GLU
1	B	47	LYS
1	B	50	LYS
1	B	117	CYS
1	B	123	LYS
1	B	141	MSE
1	B	178	LYS
1	B	182	MSE
1	B	203	SER
1	C	6	ASN
1	C	17	ARG
1	C	26	GLU
1	C	47	LYS
1	C	69[A]	SER
1	C	69[B]	SER
1	C	106	THR
1	C	121	LYS
1	C	139	LYS
1	C	141	MSE
1	C	161	ILE
1	C	167	LEU
1	C	168	LYS
1	C	182	MSE
1	C	203	SER
1	C	206	GLU
1	C	223	LEU
1	D	6	ASN
1	D	17	ARG
1	D	45	LYS
1	D	109	GLN
1	D	141	MSE
1	D	167	LEU
1	D	169	ASP
1	D	182	MSE
1	D	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	41	HIS
1	A	42	ASN
1	A	114	GLN
1	A	213	GLN
1	B	6	ASN
1	B	25	HIS
1	B	42	ASN
1	B	75	HIS
1	B	137	GLN
1	B	172	HIS
1	B	213	GLN
1	C	25	HIS
1	C	41	HIS
1	C	42	ASN
1	C	204	HIS
1	C	213	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	CRQ	A	66	1	24,25,26	2.25	8 (33%)	26,34,36	1.81	4 (15%)
1	CRQ	B	66	1	24,25,26	3.52	11 (45%)	26,34,36	2.42	8 (30%)
1	CRQ	C	66	1	24,25,26	2.30	8 (33%)	26,34,36	1.76	5 (19%)
1	CRQ	D	66	1	24,25,26	3.34	9 (37%)	26,34,36	1.95	7 (26%)

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	CRQ	A	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	B	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	C	66	1	-	0/10/32/33	0/2/2/2
1	CRQ	D	66	1	-	0/10/32/33	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRQ	CA1-N	-12.63	0.96	1.27
1	D	66	CRQ	CA1-N	-12.24	0.97	1.27
1	B	66	CRQ	OH-CZ	-4.99	1.25	1.37
1	C	66	CRQ	OH-CZ	-4.78	1.25	1.37
1	D	66	CRQ	OH-CZ	-4.37	1.26	1.37
1	A	66	CRQ	CG2-CB2	-4.22	1.38	1.46
1	A	66	CRQ	OH-CZ	-4.13	1.27	1.37
1	C	66	CRQ	CG2-CB2	-3.63	1.39	1.46
1	B	66	CRQ	CG2-CB2	-3.35	1.40	1.46
1	D	66	CRQ	CG2-CB2	-2.95	1.40	1.46
1	C	66	CRQ	CA1-N	-2.52	1.21	1.27
1	A	66	CRQ	CA3-N3	-2.11	1.42	1.47
1	C	66	CRQ	CE2-CD2	-2.02	1.35	1.38
1	B	66	CRQ	CA2-C2	2.16	1.50	1.48
1	B	66	CRQ	CB1-CA1	2.30	1.57	1.50
1	C	66	CRQ	CE2-CZ	2.31	1.43	1.38
1	D	66	CRQ	C1-N3	2.46	1.43	1.38
1	B	66	CRQ	CD1-CG2	2.51	1.44	1.39
1	A	66	CRQ	CB1-CA1	2.55	1.58	1.50
1	A	66	CRQ	CD2-CG2	2.56	1.44	1.39
1	B	66	CRQ	CD2-CG2	2.63	1.44	1.39
1	D	66	CRQ	CD2-CG2	2.64	1.44	1.39
1	D	66	CRQ	CD1-CG2	3.13	1.45	1.39
1	B	66	CRQ	C1-N3	3.19	1.44	1.38
1	A	66	CRQ	CE2-CZ	3.61	1.46	1.38
1	C	66	CRQ	CE1-CZ	3.63	1.46	1.38
1	A	66	CRQ	C1-N3	3.89	1.45	1.38
1	D	66	CRQ	CE2-CZ	3.94	1.46	1.38
1	B	66	CRQ	CE2-CZ	3.98	1.46	1.38
1	C	66	CRQ	C1-N3	4.03	1.45	1.38
1	D	66	CRQ	CE1-CZ	4.13	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRQ	CE1-CZ	4.18	1.47	1.38
1	A	66	CRQ	CE1-CZ	4.72	1.48	1.38
1	C	66	CRQ	CB2-CA2	4.81	1.39	1.35
1	D	66	CRQ	CB2-CA2	4.89	1.39	1.35
1	B	66	CRQ	CB2-CA2	5.01	1.39	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRQ	CB1-CA1-N	-5.82	105.25	125.34
1	A	66	CRQ	CB1-CA1-N	-5.66	105.80	125.34
1	D	66	CRQ	CB1-CA1-N	-4.43	110.05	125.34
1	A	66	CRQ	CE2-CZ-CE1	-2.84	114.63	119.74
1	D	66	CRQ	CE2-CZ-CE1	-2.69	114.90	119.74
1	C	66	CRQ	CE2-CZ-CE1	-2.55	115.16	119.74
1	B	66	CRQ	CE2-CZ-CE1	-2.52	115.21	119.74
1	B	66	CRQ	CB2-CA2-C2	-2.51	119.17	122.32
1	C	66	CRQ	CB2-CA2-C2	-2.43	119.27	122.32
1	D	66	CRQ	CB2-CA2-C2	-2.22	119.52	122.32
1	D	66	CRQ	CB2-CA2-N2	2.01	131.84	128.79
1	C	66	CRQ	CD1-CE1-CZ	2.02	122.17	119.88
1	B	66	CRQ	O2-C2-CA2	2.19	132.15	130.97
1	B	66	CRQ	CB2-CA2-N2	2.22	132.14	128.79
1	B	66	CRQ	CD2-CE2-CZ	2.23	122.41	119.88
1	D	66	CRQ	CD2-CE2-CZ	2.46	122.67	119.88
1	A	66	CRQ	CG2-CB2-CA2	3.01	133.69	130.19
1	A	66	CRQ	CA2-C2-N3	3.40	104.81	103.30
1	C	66	CRQ	CA2-C2-N3	4.29	105.21	103.30
1	D	66	CRQ	CA2-C2-N3	4.37	105.25	103.30
1	D	66	CRQ	CG2-CB2-CA2	4.66	135.61	130.19
1	C	66	CRQ	CG2-CB2-CA2	4.78	135.75	130.19
1	B	66	CRQ	CG2-CB2-CA2	5.98	137.14	130.19
1	B	66	CRQ	CA2-C2-N3	6.55	106.22	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRQ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRQ	1	0
1	D	66	CRQ	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	211/234 (90%)	0.03	2 (0%) 84 83	8, 14, 37, 89	0
1	B	211/234 (90%)	0.00	3 (1%) 75 75	7, 13, 32, 63	0
1	C	211/234 (90%)	0.09	1 (0%) 90 90	9, 16, 36, 67	0
1	D	211/234 (90%)	0.08	3 (1%) 75 75	9, 15, 37, 81	0
All	All	844/936 (90%)	0.05	9 (1%) 80 80	7, 15, 37, 89	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	5.9
1	D	52	GLY	4.9
1	D	6	ASN	4.7
1	D	169	ASP	4.4
1	C	6	ASN	4.2
1	B	6	ASN	3.1
1	B	169	ASP	2.2
1	A	115	ASP	2.1
1	B	52	GLY	2.1

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRQ	D	66	24/25	0.91	0.18	-	11,17,23,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CRQ	C	66	24/25	0.93	0.16	-	8,19,27,35	0
1	CRQ	B	66	24/25	0.95	0.15	-	6,14,20,34	0
1	CRQ	A	66	24/25	0.93	0.17	-	6,19,26,27	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.