



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 2BTJ / pdb_00002btj
Title : Fluorescent Protein EosFP - red form
Authors : Nar, H.; Nienhaus, K.; Wiedenmann, J.; Nienhaus, G.U.
Deposited on : 2005-06-01
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

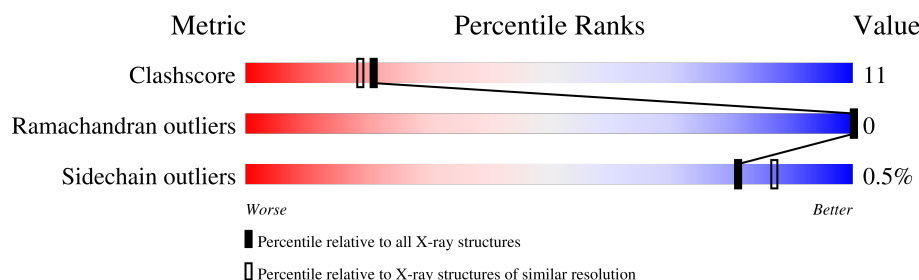
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	aa	61	84% 16%
1	bb	61	82% 18%
1	cc	61	79% 20% .
1	dd	61	85% 15%
2	A	159	75% 23% .
2	B	159	75% 24% .
2	C	159	75% 25%
2	D	159	79% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7796 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 to red photoconvertible GFP-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	aa	61	Total	C	N	O	S	13	0	0
			460	292	78	87	3			
1	bb	61	Total	C	N	O	S	13	0	0
			460	292	78	87	3			
1	cc	61	Total	C	N	O	S	13	0	0
			460	292	78	87	3			
1	dd	61	Total	C	N	O	S	13	0	0
			460	292	78	87	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aa	1	GLY	-	expression tag	UNP Q5S6Z9
aa	2	GLY	-	expression tag	UNP Q5S6Z9
bb	1	GLY	-	expression tag	UNP Q5S6Z9
bb	2	GLY	-	expression tag	UNP Q5S6Z9
cc	1	GLY	-	expression tag	UNP Q5S6Z9
cc	2	GLY	-	expression tag	UNP Q5S6Z9
dd	1	GLY	-	expression tag	UNP Q5S6Z9
dd	2	GLY	-	expression tag	UNP Q5S6Z9

- Molecule 2 is a protein called Green to red photoconvertible GFP-like protein EosFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	159	Total	C	N	O	S	10	0	0
			1315	843	225	240	7			
2	B	159	Total	C	N	O	S	7	0	0
			1315	843	225	240	7			
2	C	159	Total	C	N	O	S	10	0	0
			1315	843	225	240	7			
2	D	159	Total	C	N	O	S	5	0	0
			1315	843	225	240	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	RC7	HIS	chromophore	UNP Q5S6Z9
A	64	RC7	TYR	chromophore	UNP Q5S6Z9
A	64	RC7	GLY	chromophore	UNP Q5S6Z9
B	64	RC7	HIS	chromophore	UNP Q5S6Z9
B	64	RC7	TYR	chromophore	UNP Q5S6Z9
B	64	RC7	GLY	chromophore	UNP Q5S6Z9
C	64	RC7	HIS	chromophore	UNP Q5S6Z9
C	64	RC7	TYR	chromophore	UNP Q5S6Z9
C	64	RC7	GLY	chromophore	UNP Q5S6Z9
D	64	RC7	HIS	chromophore	UNP Q5S6Z9
D	64	RC7	TYR	chromophore	UNP Q5S6Z9
D	64	RC7	GLY	chromophore	UNP Q5S6Z9

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	176	Total O 176 176	0	0
3	B	185	Total O 185 185	0	0
3	C	173	Total O 173 173	0	0
3	D	162	Total O 162 162	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain aa: 



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain bb: 



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain cc: 



- Molecule 1: Green to red photoconvertible GFP-like protein EosFP

Chain dd: 

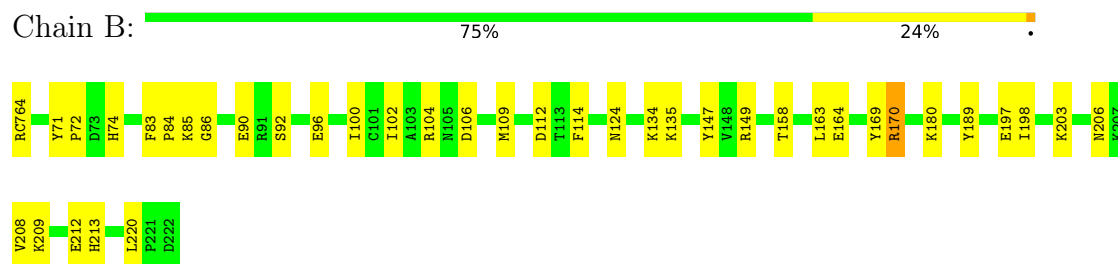


- Molecule 2: Green to red photoconvertible GFP-like protein EosFP

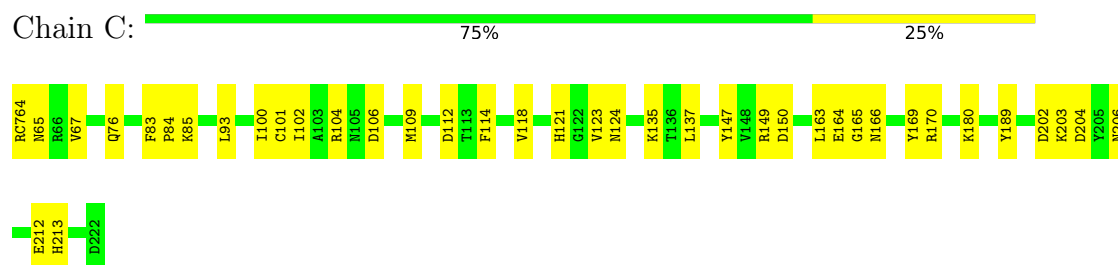
Chain A: 



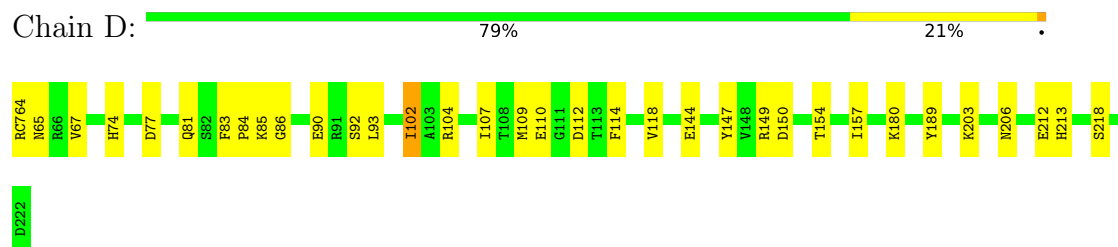
- Molecule 2: Green to red photoconvertible GFP-like protein EosFP



- Molecule 2: Green to red photoconvertible GFP-like protein EosFP



- Molecule 2: Green to red photoconvertible GFP-like protein EosFP



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.59Å 105.51Å 119.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (50.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7796	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NFA, RC7

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	aa	0.36	0/457	0.82	0/613
1	bb	0.38	0/457	0.91	1/613 (0.2%)
1	cc	0.37	0/457	0.86	1/613 (0.2%)
1	dd	0.39	0/457	0.91	3/613 (0.5%)
2	A	0.35	0/1328	0.92	6/1793 (0.3%)
2	B	0.35	0/1328	0.91	4/1793 (0.2%)
2	C	0.34	0/1328	0.90	4/1793 (0.2%)
2	D	0.35	0/1328	0.92	3/1793 (0.2%)
All	All	0.36	0/7140	0.90	22/9624 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bb	58	THR	N-CA-C	8.54	121.66	111.33
1	dd	58	THR	N-CA-C	8.27	121.04	111.11
1	cc	58	THR	N-CA-C	7.45	120.05	111.11
2	B	124	ASN	N-CA-C	6.20	120.43	112.86
2	C	124	ASN	N-CA-C	5.71	119.83	112.86
2	C	170	ARG	N-CA-C	5.64	118.83	110.48
2	A	118	VAL	N-CA-C	5.59	116.64	108.53
2	C	206	ASN	N-CA-C	-5.56	106.00	112.89
2	B	170	ARG	N-CA-C	5.50	118.62	110.48
2	D	118	VAL	N-CA-C	5.44	116.42	108.53
2	A	67	VAL	N-CA-C	-5.44	104.29	111.09
1	dd	32	LYS	CA-C-N	5.35	124.80	119.24
1	dd	32	LYS	C-N-CA	5.35	124.80	119.24
2	B	206	ASN	N-CA-C	-5.18	106.81	113.23
2	B	96	GLU	N-CA-C	5.12	118.63	112.38
2	A	203	LYS	N-CA-C	5.10	117.23	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	79	PHE	N-CA-C	5.06	116.61	111.14
2	A	198	ILE	N-CA-C	-5.06	99.83	107.73
2	A	124	ASN	N-CA-C	5.06	119.03	112.86
2	C	118	VAL	N-CA-C	5.05	115.75	108.48
2	D	107	ILE	N-CA-C	5.03	115.10	107.80
2	D	206	ASN	N-CA-C	-5.03	106.65	112.89

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	aa	460	0	451	11	0
1	bb	460	0	451	12	0
1	cc	460	0	451	12	0
1	dd	460	0	451	9	0
2	A	1315	0	1252	31	0
2	B	1315	0	1252	35	0
2	C	1315	0	1252	34	0
2	D	1315	0	1252	37	0
3	A	176	0	0	2	0
3	B	185	0	0	15	0
3	C	173	0	0	10	0
3	D	162	0	0	15	0
All	All	7796	0	6812	150	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 11.

All (150) 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:cc:8:MET:HE2	2:C:109:MET:HE2	1.49	0.91
1:bb:8:MET:HE2	2:B:109:MET:HE2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:dd:5:LYS:HG2	3:D:2078:HOH:O	1.75	0.85
2:B:203:LYS:HE2	2:B:203:LYS:N	1.98	0.79
1:bb:3:ALA:HB1	3:B:2078:HOH:O	1.84	0.78
1:cc:49:PRO:HB3	2:C:204:ASP:HB3	1.66	0.76
2:B:112:ASP:HB2	3:B:2092:HOH:O	1.85	0.76
2:C:112:ASP:HB2	3:C:2086:HOH:O	1.85	0.74
2:D:112:ASP:HB2	3:D:2081:HOH:O	1.86	0.74
2:D:110:GLU:HG2	3:D:2076:HOH:O	1.87	0.73
1:aa:8:MET:HE2	2:A:109:MET:HE2	1.70	0.72
1:cc:4:ILE:HG12	2:C:109:MET:HE1	1.71	0.72
1:cc:8:MET:CE	2:C:109:MET:HE2	2.21	0.71
2:A:81:GLN:HE21	2:A:81:GLN:HA	1.54	0.70
1:aa:8:MET:CE	2:A:109:MET:HE2	2.22	0.68
1:cc:9:LYS:HG3	3:C:2006:HOH:O	1.92	0.68
2:B:203:LYS:HE2	2:B:203:LYS:H	1.58	0.67
2:A:137:LEU:HD21	2:A:164:GLU:HG2	1.76	0.67
1:bb:7:ASP:HB2	3:B:2004:HOH:O	1.95	0.66
2:A:102:ILE:HD13	2:D:102:ILE:HD13	1.78	0.66
2:A:83:PHE:HB3	2:A:84:PRO:HA	1.78	0.66
1:bb:28:ASP:HB2	3:B:2025:HOH:O	1.95	0.65
2:B:100:ILE:HG22	2:C:102:ILE:HD11	1.79	0.65
2:D:203:LYS:NZ	3:D:2145:HOH:O	2.29	0.64
2:C:203:LYS:HD3	2:C:203:LYS:N	2.13	0.63
2:C:106:ASP:HB3	3:C:2136:HOH:O	1.99	0.63
2:B:104:ARG:HH22	2:B:106:ASP:CG	2.07	0.63
2:A:149:ARG:HG3	3:A:2104:HOH:O	1.98	0.62
2:B:83:PHE:HB3	2:B:84:PRO:HA	1.80	0.62
2:B:135:LYS:HE3	3:B:2102:HOH:O	1.99	0.62
1:dd:8:MET:HE2	2:D:109:MET:HE2	1.81	0.62
2:C:109:MET:HE3	2:C:114:PHE:CE1	2.35	0.62
1:bb:7:ASP:HB2	3:B:2001:HOH:O	2.00	0.61
2:A:106:ASP:HB3	3:A:2130:HOH:O	2.00	0.61
2:B:164:GLU:HB2	3:B:2125:HOH:O	2.00	0.60
2:D:109:MET:HE3	2:D:114:PHE:CE1	2.37	0.60
2:B:85:LYS:HG3	2:B:180:LYS:HB2	1.82	0.60
2:A:150:ASP:HB3	3:D:2087:HOH:O	2.03	0.59
2:C:203:LYS:HE2	3:C:2152:HOH:O	2.02	0.58
2:C:203:LYS:HD3	2:C:203:LYS:H	1.69	0.58
1:bb:8:MET:CE	2:B:109:MET:HE2	2.31	0.57
2:B:109:MET:HE3	2:B:114:PHE:CE1	2.39	0.57
1:aa:12:LEU:C	1:aa:12:LEU:HD23	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:dd:12:LEU:C	1:dd:12:LEU:HD23	2.30	0.57
2:C:204:ASP:HB2	3:C:2151:HOH:O	2.05	0.56
2:A:203:LYS:N	2:A:203:LYS:HE2	2.20	0.56
2:C:83:PHE:HB3	2:C:84:PRO:HA	1.87	0.56
2:A:203:LYS:HE2	2:A:203:LYS:H	1.70	0.56
1:dd:26:ASP:OD1	1:dd:45:LYS:HE3	2.06	0.56
2:D:149:ARG:HG2	3:D:2106:HOH:O	2.03	0.56
2:B:198:ILE:HG23	2:B:208:VAL:HG13	1.87	0.56
2:D:65:ASN:OD1	2:D:67:VAL:HG23	2.06	0.56
2:A:123:VAL:HB	2:D:90:GLU:HB3	1.89	0.55
3:B:2100:HOH:O	2:C:150:ASP:HB3	2.06	0.55
1:dd:8:MET:CE	2:D:109:MET:HE2	2.37	0.55
2:C:202:ASP:HB2	3:C:2152:HOH:O	2.08	0.54
2:C:135:LYS:HE2	2:C:164:GLU:HB2	1.89	0.54
2:A:101:CYS:O	2:A:102:ILE:HD12	2.07	0.54
2:D:147:TYR:HB3	2:D:189:TYR:CD1	2.43	0.53
2:B:90:GLU:HB3	2:C:123:VAL:HB	1.91	0.53
3:B:2013:HOH:O	2:C:104:ARG:HD3	2.09	0.53
2:A:100:ILE:HD12	2:D:92:SER:HB2	1.91	0.53
1:aa:4:ILE:HG12	2:A:109:MET:HE1	1.91	0.52
2:B:92:SER:HB2	2:C:100:ILE:HD12	1.91	0.52
1:bb:12:LEU:C	1:bb:12:LEU:HD23	2.34	0.52
2:D:83:PHE:HB3	2:D:84:PRO:HA	1.92	0.52
2:A:100:ILE:HD12	2:D:92:SER:CB	2.40	0.52
2:A:109:MET:HE3	2:A:114:PHE:CE1	2.45	0.52
2:C:203:LYS:H	2:C:203:LYS:CD	2.20	0.52
1:dd:12:LEU:HD23	1:dd:13:ARG:N	2.24	0.52
2:D:109:MET:HG2	2:D:110:GLU:N	2.24	0.52
2:D:74:HIS:HE1	2:D:218:SER:OG	1.94	0.51
2:B:147:TYR:HB3	2:B:189:TYR:CD1	2.46	0.51
2:C:147:TYR:HB3	2:C:189:TYR:CD1	2.46	0.51
1:cc:49:PRO:CB	2:C:204:ASP:HB3	2.38	0.50
2:B:203:LYS:H	2:B:203:LYS:CE	2.22	0.50
1:cc:12:LEU:C	1:cc:12:LEU:HD23	2.36	0.50
2:D:85:LYS:O	2:D:180:LYS:HD2	2.12	0.50
1:bb:5:LYS:HB2	1:bb:8:MET:SD	2.51	0.49
1:aa:19:ASN:HA	2:D:90:GLU:OE2	2.11	0.49
2:C:149:ARG:HG2	3:C:2114:HOH:O	2.13	0.49
2:C:85:LYS:HG3	2:C:180:LYS:HB2	1.95	0.49
2:D:77:ASP:O	2:D:81:GLN:HG2	2.12	0.49
2:A:165:GLY:O	2:A:166:ASN:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:LEU:HB3	3:B:2183:HOH:O	2.13	0.48
2:B:90:GLU:OE2	1:cc:19:ASN:HA	2.12	0.48
2:D:86:GLY:C	2:D:180:LYS:HG3	2.38	0.48
2:B:102:ILE:HG13	3:B:2088:HOH:O	2.14	0.47
2:A:74:HIS:HE1	2:A:218:SER:OG	1.97	0.47
2:D:86:GLY:O	2:D:180:LYS:HG3	2.14	0.47
2:A:198:ILE:HG23	2:A:208:VAL:HG13	1.95	0.47
2:C:165:GLY:O	2:C:166:ASN:HB2	2.14	0.47
2:B:212:GLU:HG2	2:B:213:HIS:N	2.28	0.47
2:D:150:ASP:HA	3:D:2109:HOH:O	2.15	0.47
2:D:81:GLN:HE21	2:D:81:GLN:HA	1.80	0.46
1:bb:5:LYS:HD3	3:B:2091:HOH:O	2.15	0.46
2:D:203:LYS:HB2	3:D:2146:HOH:O	2.15	0.46
1:bb:50:LEU:O	2:B:134:LYS:HE2	2.16	0.46
2:B:86:GLY:HA3	2:B:180:LYS:HE2	1.98	0.46
2:D:93:LEU:HD12	2:D:93:LEU:N	2.31	0.46
2:D:144:GLU:HA	2:D:157:ILE:HG12	1.97	0.45
1:aa:16:GLY:HA3	2:A:120:PHE:O	2.17	0.45
1:bb:4:ILE:HG12	2:B:109:MET:HE1	1.99	0.45
2:B:74:HIS:HD2	3:B:2062:HOH:O	1.98	0.45
2:D:149:ARG:HG3	3:D:2104:HOH:O	2.17	0.45
2:B:92:SER:CB	2:C:100:ILE:HD12	2.46	0.45
2:B:158:THR:HG23	2:B:170:ARG:CZ	2.47	0.45
2:A:87:TYR:HA	2:A:180:LYS:HG3	1.98	0.45
2:A:158:THR:HG23	2:A:170:ARG:CZ	2.48	0.44
2:C:93:LEU:HB2	2:C:101:CYS:HB2	1.99	0.44
2:C:213:HIS:HE1	3:C:2054:HOH:O	2.00	0.44
2:D:112:ASP:HA	3:D:2079:HOH:O	2.16	0.44
2:C:163:LEU:HD11	2:C:169:TYR:HB2	1.99	0.44
2:B:102:ILE:HD11	2:C:121:HIS:HB2	2.00	0.44
2:C:137:LEU:HD21	2:C:164:GLU:HG2	2.00	0.44
2:D:212:GLU:HG2	2:D:213:HIS:N	2.33	0.44
1:aa:33:PRO:HB2	2:A:80:LYS:HE3	2.00	0.43
2:B:163:LEU:HD11	2:B:169:TYR:HB2	2.01	0.43
1:aa:5:LYS:N	1:aa:5:LYS:HD2	2.34	0.43
2:B:104:ARG:NH2	2:B:106:ASP:OD2	2.52	0.43
1:aa:58:THR:HA	1:aa:61:NFA:HD1	2.00	0.43
1:cc:28:ASP:HB2	3:C:2018:HOH:O	2.19	0.43
2:D:85:LYS:HG3	2:D:180:LYS:HB2	2.02	0.42
1:cc:17:ASN:HA	1:cc:21:HIS:O	2.19	0.42
2:D:149:ARG:HD2	3:D:2042:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:8:MET:HE1	2:A:109:MET:HE2	1.99	0.42
2:A:181:GLU:HG2	2:A:182:LYS:O	2.19	0.42
2:B:71:TYR:HA	2:B:72:PRO:HD3	1.85	0.42
2:B:104:ARG:HD2	3:C:2092:HOH:O	2.19	0.42
2:A:123:VAL:HG22	2:D:102:ILE:HG13	2.01	0.41
2:A:139:TRP:CE3	2:A:159:MET:HE3	2.56	0.41
2:D:203:LYS:HG2	3:D:2056:HOH:O	2.19	0.41
1:cc:26:ASP:OD1	1:cc:45:LYS:HE3	2.21	0.41
2:B:209:LYS:HD2	3:B:2036:HOH:O	2.21	0.41
1:cc:58:THR:HA	1:cc:61:NFA:HD1	2.03	0.41
2:C:76:GLN:HA	2:C:76:GLN:HE21	1.86	0.41
2:C:212:GLU:HG2	2:C:213:HIS:N	2.36	0.41
2:A:85:LYS:O	2:A:180:LYS:HD2	2.20	0.41
1:aa:12:LEU:HD23	1:aa:13:ARG:N	2.35	0.41
2:B:72:PRO:HB2	2:B:74:HIS:CD2	2.55	0.41
2:C:65:ASN:OD1	2:C:67:VAL:HB	2.21	0.41
1:dd:4:ILE:HG12	2:D:109:MET:HE1	2.03	0.41
2:A:83:PHE:CE2	2:A:86:GLY:HA2	2.56	0.41
1:bb:21:HIS:CD2	1:bb:51:PRO:HG3	2.56	0.41
2:D:154:THR:HG21	3:D:2105:HOH:O	2.19	0.41
1:dd:13:ARG:HD2	3:D:2007:HOH:O	2.22	0.40
2:A:123:VAL:CG2	2:D:102:ILE:HG13	2.52	0.40
2:B:149:ARG:HG3	3:B:2117:HOH:O	2.21	0.40
1:dd:5:LYS:HD3	3:D:2079:HOH:O	2.21	0.40
2:D:104:ARG:CZ	2:D:104:ARG:HB2	2.51	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	aa	59/61 (97%)	58 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	bb	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
1	cc	59/61 (97%)	59 (100%)	0	0	100	100
1	dd	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
2	A	156/159 (98%)	153 (98%)	3 (2%)	0	100	100
2	B	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
2	C	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
2	D	156/159 (98%)	151 (97%)	5 (3%)	0	100	100
All	All	860/880 (98%)	840 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	aa	47/47 (100%)	47 (100%)	0	100	100
1	bb	47/47 (100%)	47 (100%)	0	100	100
1	cc	47/47 (100%)	47 (100%)	0	100	100
1	dd	47/47 (100%)	47 (100%)	0	100	100
2	A	138/138 (100%)	136 (99%)	2 (1%)	59	66
2	B	138/138 (100%)	137 (99%)	1 (1%)	76	82
2	C	138/138 (100%)	138 (100%)	0	100	100
2	D	138/138 (100%)	137 (99%)	1 (1%)	76	82
All	All	740/740 (100%)	736 (100%)	4 (0%)	81	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	76	GLN
2	A	81	GLN

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Mol	Chain	Res	Type
2	B	197	GLU
2	D	102	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	aa	22	HIS
1	aa	38	GLN
2	A	74	HIS
2	A	76	GLN
2	A	81	GLN
2	A	206	ASN
2	A	213	HIS
1	bb	21	HIS
1	bb	22	HIS
2	B	74	HIS
2	B	76	GLN
2	B	81	GLN
2	B	121	HIS
2	B	213	HIS
1	cc	22	HIS
2	C	76	GLN
2	C	81	GLN
2	C	213	HIS
1	dd	22	HIS
2	D	74	HIS
2	D	76	GLN
2	D	81	GLN
2	D	121	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	NFA	aa	61	1	12,12,12	0.47	0	15,15,15	0.64	0
2	RC7	D	64	2	26,26,27	1.50	5 (19%)	33,35,37	2.09	10 (30%)
2	RC7	A	64	2	26,26,27	1.53	4 (15%)	33,35,37	2.12	10 (30%)
1	NFA	cc	61	1	12,12,12	0.53	0	15,15,15	0.50	0
2	RC7	C	64	2	26,26,27	1.50	5 (19%)	33,35,37	2.05	10 (30%)
1	NFA	dd	61	1	12,12,12	0.43	0	15,15,15	0.47	0
1	NFA	bb	61	1	12,12,12	0.53	0	15,15,15	0.36	0
2	RC7	B	64	2	26,26,27	1.51	5 (19%)	33,35,37	1.97	10 (30%)

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	NFA	aa	61	1	-	4/8/8/8	0/1/1/1
2	RC7	D	64	2	-	1/11/28/29	0/3/3/3
2	RC7	A	64	2	-	1/11/28/29	0/3/3/3
1	NFA	cc	61	1	-	3/8/8/8	0/1/1/1
2	RC7	C	64	2	-	1/11/28/29	0/3/3/3
1	NFA	dd	61	1	-	2/8/8/8	0/1/1/1
1	NFA	bb	61	1	-	4/8/8/8	0/1/1/1
2	RC7	B	64	2	-	1/11/28/29	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	64	RC7	CB2-CA2	4.09	1.39	1.35
2	C	64	RC7	CB2-CA2	4.09	1.39	1.35
2	B	64	RC7	CB2-CA2	3.93	1.39	1.35
2	D	64	RC7	CB2-CA2	3.88	1.38	1.35
2	C	64	RC7	CG1-ND1	-3.60	1.32	1.39
2	D	64	RC7	CG1-ND1	-3.59	1.32	1.39
2	B	64	RC7	CG1-ND1	-3.55	1.32	1.39
2	A	64	RC7	CG1-ND1	-3.50	1.32	1.39
2	A	64	RC7	CD2-CG2	2.55	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	64	RC7	CD2-CG2	2.40	1.44	1.39
2	D	64	RC7	CE2-CZ	2.31	1.43	1.39
2	B	64	RC7	CD2-CG2	2.30	1.44	1.39
2	C	64	RC7	CD2-CG2	2.23	1.44	1.39
2	C	64	RC7	CE2-CZ	2.22	1.43	1.39
2	B	64	RC7	CD1-CG2	2.18	1.43	1.39
2	D	64	RC7	CD1-CG2	2.16	1.43	1.39
2	C	64	RC7	CD1-CG2	2.13	1.43	1.39
2	B	64	RC7	CE2-CZ	2.12	1.43	1.39
2	A	64	RC7	CE2-CZ	2.04	1.42	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	64	RC7	O2-C2-CA2	-6.74	126.72	131.02
2	D	64	RC7	O2-C2-CA2	-6.44	126.91	131.02
2	C	64	RC7	O2-C2-CA2	-6.34	126.97	131.02
2	B	64	RC7	O2-C2-CA2	-6.14	127.10	131.02
2	A	64	RC7	N3-C1-N2	-4.31	110.77	112.87
2	C	64	RC7	N3-C1-N2	-4.15	110.84	112.87
2	B	64	RC7	N3-C1-N2	-3.99	110.92	112.87
2	D	64	RC7	N3-C1-N2	-3.97	110.93	112.87
2	C	64	RC7	CA2-N2-C1	3.88	109.22	105.57
2	A	64	RC7	CA2-N2-C1	3.86	109.20	105.57
2	D	64	RC7	CA2-N2-C1	3.83	109.18	105.57
2	D	64	RC7	CG2-CB2-CA2	3.46	133.98	129.87
2	B	64	RC7	CA2-N2-C1	3.37	108.74	105.57
2	D	64	RC7	C2-CA2-N2	-3.20	106.66	108.95
2	A	64	RC7	C2-CA2-N2	-3.19	106.67	108.95
2	C	64	RC7	C2-CA2-N2	-3.17	106.68	108.95
2	C	64	RC7	CG2-CB2-CA2	3.03	133.47	129.87
2	B	64	RC7	C2-CA2-N2	-2.85	106.91	108.95
2	A	64	RC7	CG2-CB2-CA2	2.80	133.19	129.87
2	D	64	RC7	C3-CA3-N3	2.79	118.78	112.43
2	B	64	RC7	CG2-CB2-CA2	2.73	133.12	129.87
2	A	64	RC7	C3-CA3-N3	2.63	118.41	112.43
2	B	64	RC7	C3-CA3-N3	2.61	118.38	112.43
2	C	64	RC7	CE3-ND1-CG1	2.61	109.32	104.97
2	A	64	RC7	CE3-ND1-CG1	2.57	109.26	104.97
2	B	64	RC7	CE3-ND1-CG1	2.50	109.13	104.97
2	D	64	RC7	CE3-ND1-CG1	2.47	109.09	104.97
2	A	64	RC7	CB2-CA2-C2	2.44	125.31	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	RC7	CA1-CB1-CG1	-2.40	118.94	129.21
2	D	64	RC7	CA1-CB1-CG1	-2.38	119.03	129.21
2	C	64	RC7	CA1-CB1-CG1	-2.37	119.07	129.21
2	A	64	RC7	CA1-CB1-CG1	-2.33	119.24	129.21
2	A	64	RC7	CA2-C2-N3	2.30	105.44	103.50
2	C	64	RC7	CB2-CA2-C2	2.26	125.09	122.36
2	B	64	RC7	CA2-C2-N3	2.23	105.37	103.50
2	D	64	RC7	CA2-C2-N3	2.22	105.37	103.50
2	C	64	RC7	C3-CA3-N3	2.21	117.46	112.43
2	C	64	RC7	CA2-C2-N3	2.16	105.31	103.50
2	B	64	RC7	CB2-CA2-C2	2.10	124.91	122.36
2	D	64	RC7	CB2-CA2-C2	2.10	124.90	122.36

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	aa	61	NFA	NXT-C-CA-N
1	aa	61	NFA	O-C-CA-CB
2	A	64	RC7	C3-CA3-N3-C2
1	bb	61	NFA	O-C-CA-N
1	bb	61	NFA	NXT-C-CA-N
2	B	64	RC7	C3-CA3-N3-C2
1	cc	61	NFA	O-C-CA-N
1	cc	61	NFA	NXT-C-CA-N
2	C	64	RC7	C3-CA3-N3-C2
1	dd	61	NFA	O-C-CA-N
1	dd	61	NFA	NXT-C-CA-N
2	D	64	RC7	C3-CA3-N3-C2
1	aa	61	NFA	NXT-C-CA-CB
1	aa	61	NFA	O-C-CA-N
1	bb	61	NFA	O-C-CA-CB
1	bb	61	NFA	NXT-C-CA-CB
1	cc	61	NFA	NXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	aa	61	NFA	1	0
1	cc	61	NFA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.