



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2025 – 12:18 PM EDT

PDB ID : 9DVE / pdb_00009dve
Title : X-ray crystal structure of Kohinoor reversibly switchable fluorescent protein
Authors : Richardson, B.C.; He, Y.; Iuliano, J.N.; Woroniecka, H.A.; French, J.B.
Deposited on : 2024-10-07
Resolution : 2.15 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

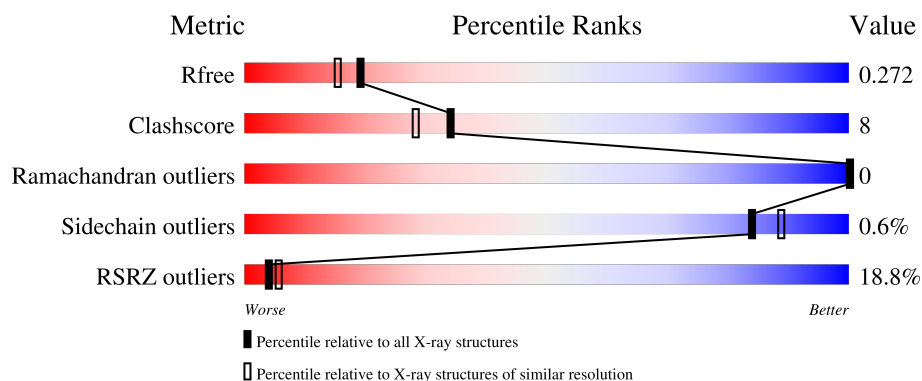
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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 $\leq 5\%$. 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	226	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>5%</div> </div> </div>
1	B	226	<div> <div>12%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>•</div> </div> </div>
1	C	226	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>
1	D	226	<div> <div>39%</div> <div> <div></div> <div>70%</div> <div>11%</div> <div>•</div> <div>18%</div> </div> </div>

2 Entry composition [i](#)

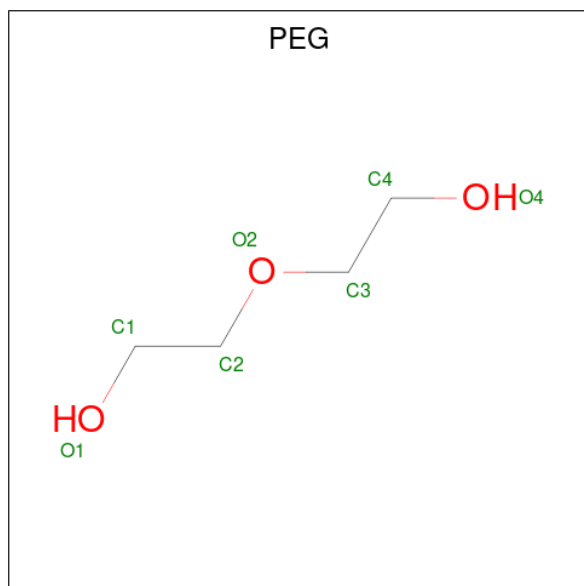
There are 3 unique types of molecules in this entry. The entry contains 12333 atoms, of which 5791 are hydrogens and 0 are deuteriums.

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 Kohinoor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	H	N	O	S	0	0	0
			3302	1085	1603	286	318	10			
1	B	217	Total	C	H	N	O	S	0	0	0
			3236	1073	1553	285	315	10			
1	C	213	Total	C	H	N	O	S	0	0	0
			3196	1060	1529	283	314	10			
1	D	185	Total	C	H	N	O	S	0	0	0
			2426	837	1096	227	258	8			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		

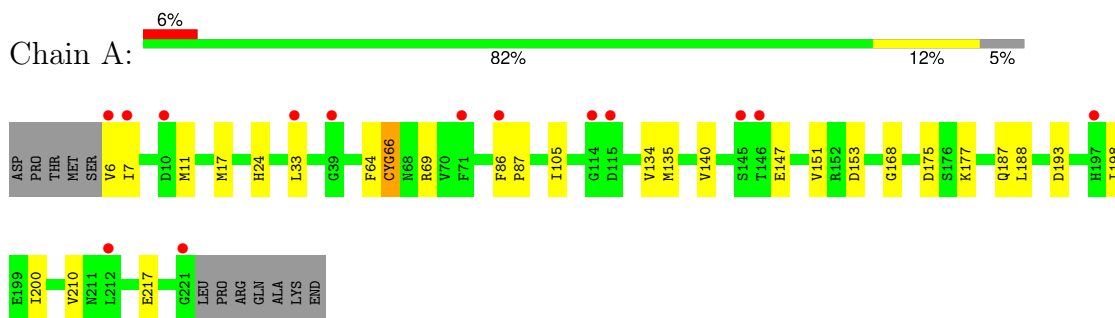
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	37	Total 37	O 37	0	0
3	C	44	Total 44	O 44	0	0
3	D	22	Total 22	O 22	0	0

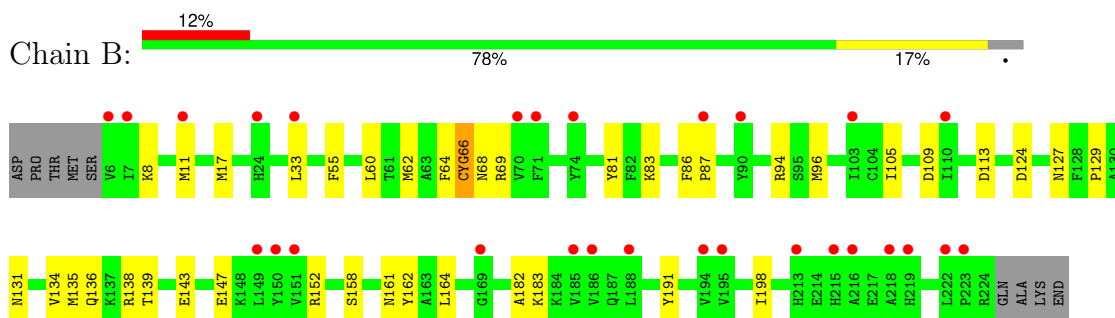
3 Residue-property plots [i](#)

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 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.

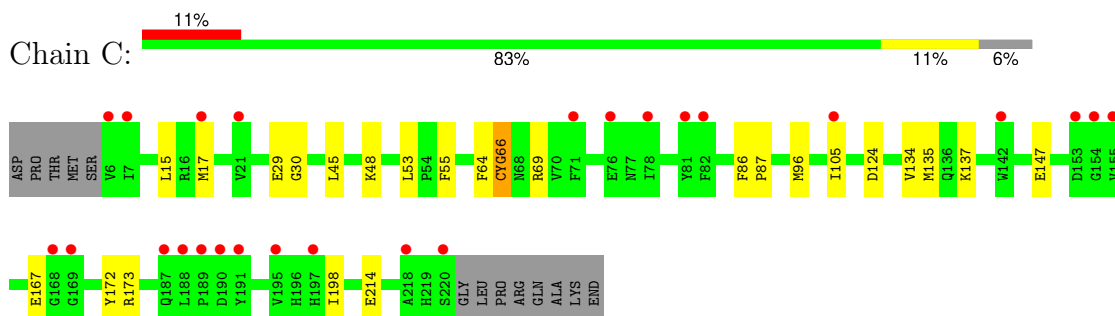
- Molecule 1: Kohinoor



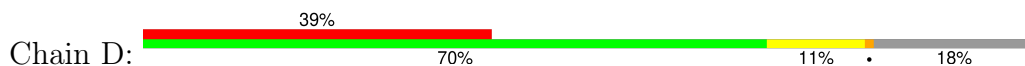
- Molecule 1: Kohinoor

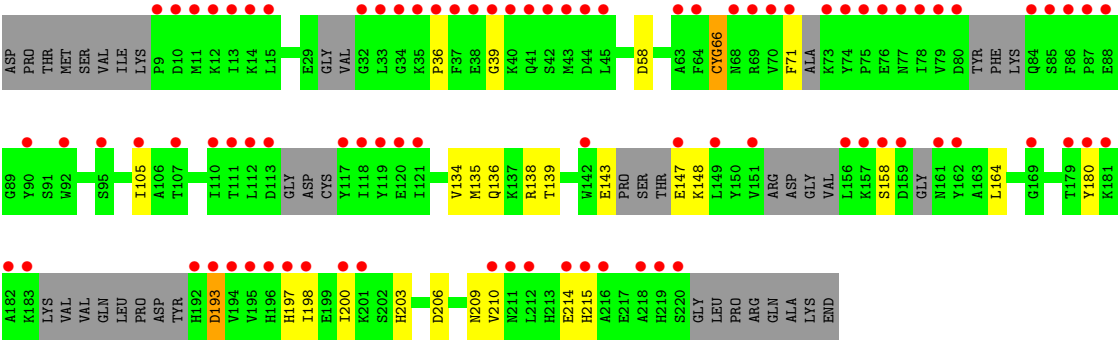


- Molecule 1: Kohinoor



- Molecule 1: Kohinoor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.53Å 73.63Å 93.22Å 90.00° 115.86° 90.00°	Depositor
Resolution (Å)	83.89 – 2.15 83.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (83.89-2.15) 96.0 (83.88-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.244 , 0.272 0.245 , 0.272	Depositor DCC
R_{free} test set	2211 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12333	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.14	0/1722	0.37	0/2328
1	B	0.17	0/1705	0.36	0/2311
1	C	0.16	0/1690	0.38	0/2291
1	D	0.19	0/1333	0.40	0/1805
All	All	0.16	0/6450	0.38	0/8735

There are no bond length outliers.

There are no bond angle outliers.

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	1699	1603	1611	22	0
1	B	1683	1553	1562	37	0
1	C	1667	1529	1536	19	0
1	D	1330	1096	1098	17	0
2	A	7	10	10	0	0
3	A	53	0	0	7	0
3	B	37	0	0	12	0
3	C	44	0	0	6	0
3	D	22	0	0	2	0
All	All	6542	5791	5817	92	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 8.

All (92) 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:B:62:MET:HE1	1:B:162:TYR:CE2	2.01	0.95
1:A:193:ASP:OD1	3:A:401:HOH:O	1.86	0.92
1:C:96:MET:SD	3:C:343:HOH:O	2.35	0.84
1:B:136:GLN:OE1	1:B:138:ARG:NH1	2.13	0.82
1:B:113:ASP:OD2	3:B:301:HOH:O	1.97	0.81
1:D:206:ASP:OD2	3:D:301:HOH:O	1.98	0.80
1:B:143:GLU:O	3:B:302:HOH:O	1.99	0.79
1:B:161:ASN:ND2	3:B:305:HOH:O	2.13	0.75
1:B:152:ARG:O	3:B:303:HOH:O	2.06	0.73
1:B:62:MET:HE3	1:B:66:GYC:CD1	2.20	0.72
1:D:143:GLU:OE2	3:D:302:HOH:O	2.10	0.69
1:A:24:HIS:NE2	3:A:405:HOH:O	2.24	0.69
1:B:129:PRO:O	3:B:304:HOH:O	2.10	0.68
1:B:127:ASN:O	3:B:306:HOH:O	2.13	0.65
1:C:69:ARG:NH1	1:C:147:GLU:OE1	2.29	0.65
1:A:140:VAL:O	3:A:403:HOH:O	2.13	0.65
1:B:124:ASP:OD1	3:B:307:HOH:O	2.15	0.65
1:D:66:GYC:HE2	1:D:198:ILE:HB	1.78	0.64
1:A:66:GYC:HE2	1:A:198:ILE:HB	1.78	0.64
1:A:7:ILE:HA	1:A:11:MET:HE2	1.79	0.63
1:A:175:ASP:CG	3:A:404:HOH:O	2.44	0.61
1:D:134:VAL:HG12	1:D:135:MET:HE2	1.82	0.61
1:A:168:GLY:N	3:A:402:HOH:O	1.93	0.61
1:B:69:ARG:NH1	1:B:147:GLU:OE1	2.33	0.60
1:C:66:GYC:HE2	1:C:198:ILE:HB	1.82	0.60
1:B:66:GYC:HE2	1:B:198:ILE:HB	1.82	0.60
1:A:177:LYS:NZ	3:A:404:HOH:O	2.33	0.60
1:A:69:ARG:NH1	1:A:147:GLU:OE1	2.35	0.59
1:C:214:GLU:OE2	3:C:302:HOH:O	2.17	0.59
1:C:29:GLU:OE1	1:C:48:LYS:NZ	2.35	0.58
1:A:175:ASP:OD2	3:A:404:HOH:O	2.17	0.58
1:B:68:ASN:N	3:B:311:HOH:O	2.37	0.57
1:C:173:ARG:NH2	3:C:304:HOH:O	2.23	0.57
1:C:172:TYR:OH	3:C:303:HOH:O	2.18	0.56
1:B:66:GYC:HD2	1:B:66:GYC:N2	2.22	0.55
1:C:66:GYC:HD2	1:C:66:GYC:N2	2.22	0.54
1:A:66:GYC:HD2	1:A:66:GYC:N2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ARG:NE	3:C:304:HOH:O	2.26	0.53
1:A:105:ILE:HG12	1:D:105:ILE:HD12	1.90	0.52
1:D:197:HIS:O	1:D:214:GLU:HA	2.11	0.52
1:B:62:MET:HE1	1:B:162:TYR:CD2	2.45	0.51
1:B:131:ASN:OD1	3:B:308:HOH:O	2.19	0.51
1:D:136:GLN:HB2	1:D:138:ARG:HD3	1.93	0.51
1:D:193:ASP:N	1:D:193:ASP:OD1	2.44	0.51
1:A:151:VAL:HG11	1:A:188:LEU:HD13	1.92	0.50
1:B:62:MET:HE3	1:B:66:GYC:CE1	2.42	0.49
1:A:153:ASP:O	1:B:191:TYR:CD1	2.65	0.49
1:B:55:PHE:HE1	1:B:60:LEU:HD11	1.77	0.49
1:B:96:MET:SD	3:B:337:HOH:O	2.60	0.49
1:A:66:GYC:N2	1:A:66:GYC:CD2	2.77	0.47
1:A:11:MET:O	1:A:33:LEU:HD12	2.15	0.47
1:C:66:GYC:N2	1:C:66:GYC:CD2	2.77	0.47
1:B:81:TYR:OH	1:B:182:ALA:N	2.48	0.47
1:A:134:VAL:HG12	1:A:135:MET:HE2	1.97	0.46
1:B:66:GYC:N2	1:B:66:GYC:CD2	2.77	0.46
1:B:86:PHE:HB3	1:B:87:PRO:HA	1.98	0.46
1:C:30:GLY:HA3	1:C:45:LEU:HD23	1.98	0.46
1:C:124:ASP:HB3	3:C:305:HOH:O	2.16	0.45
1:B:109:ASP:OD1	1:B:183:LYS:NZ	2.43	0.45
1:B:94:ARG:HD3	1:B:96:MET:HE3	1.98	0.45
1:C:17:MET:HE3	1:C:64:PHE:CE1	2.52	0.45
1:C:134:VAL:HG12	1:C:135:MET:HE2	1.98	0.45
1:D:66:GYC:N2	1:D:66:GYC:HD2	2.32	0.45
1:D:58:ASP:OD2	1:D:139:THR:OG1	2.32	0.44
1:C:86:PHE:HB3	1:C:87:PRO:HA	1.98	0.44
1:B:62:MET:SD	1:B:96:MET:HE1	2.58	0.44
1:D:200:ILE:HG23	1:D:210:VAL:HG13	1.99	0.44
1:B:147:GLU:OE2	1:B:158:SER:OG	2.26	0.43
1:C:55:PHE:HB3	1:C:135:MET:HE1	2.00	0.43
1:B:105:ILE:HG12	1:C:105:ILE:HD12	2.00	0.43
1:A:86:PHE:HB3	1:A:87:PRO:HA	2.01	0.43
1:D:203:HIS:HA	1:D:209:ASN:O	2.17	0.43
1:B:113:ASP:CG	3:B:301:HOH:O	2.51	0.43
1:C:15:LEU:HD12	1:C:15:LEU:C	2.44	0.43
1:D:147:GLU:OE2	1:D:180:TYR:OH	2.36	0.43
1:B:134:VAL:HG12	1:B:135:MET:HE2	2.00	0.42
1:C:53:LEU:O	1:C:137:LYS:NZ	2.45	0.42
1:D:139:THR:HB	1:D:164:LEU:HD21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:THR:HB	1:B:164:LEU:HD21	2.02	0.42
1:B:81:TYR:CZ	1:B:182:ALA:HB2	2.54	0.42
1:B:17:MET:HE3	1:B:64:PHE:CE1	2.55	0.42
1:A:6:VAL:O	1:A:6:VAL:HG13	2.20	0.42
1:D:148:LYS:O	1:D:158:SER:HA	2.20	0.41
1:B:55:PHE:CE1	1:B:60:LEU:HD11	2.55	0.41
1:A:17:MET:HE3	1:A:64:PHE:CE1	2.55	0.41
1:A:6:VAL:O	1:A:6:VAL:HG22	2.21	0.41
1:B:8:LYS:N	1:B:11:MET:HE3	2.36	0.41
1:D:39:GLY:O	1:D:215:HIS:HA	2.20	0.40
1:B:33:LEU:HD12	1:B:33:LEU:C	2.46	0.40
1:D:36:PRO:HA	1:D:71:PHE:HA	2.03	0.40
1:B:83:LYS:NZ	3:B:313:HOH:O	2.51	0.40
1:A:200:ILE:HG23	1:A:210:VAL:HG13	2.03	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	209/226 (92%)	207 (99%)	2 (1%)	0	100	100
1	B	212/226 (94%)	205 (97%)	7 (3%)	0	100	100
1	C	208/226 (92%)	205 (99%)	3 (1%)	0	100	100
1	D	164/226 (73%)	163 (99%)	1 (1%)	0	100	100
All	All	793/904 (88%)	780 (98%)	13 (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	A	177/192 (92%)	175 (99%)	2 (1%)	70	75
1	B	169/192 (88%)	169 (100%)	0	100	100
1	C	169/192 (88%)	168 (99%)	1 (1%)	84	89
1	D	116/192 (60%)	115 (99%)	1 (1%)	75	81
All	All	631/768 (82%)	627 (99%)	4 (1%)	84	89

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

Mol	Chain	Res	Type
1	A	187	GLN
1	A	217	GLU
1	C	167	GLU
1	D	193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	HIS
1	A	211	ASN

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	GYC	D	66	1	21,22,23	0.58	0	26,30,32	1.28	3 (11%)
1	GYC	C	66	1	21,22,23	3.13	7 (33%)	26,30,32	7.31	13 (50%)
1	GYC	A	66	1	21,22,23	3.12	7 (33%)	26,30,32	7.31	13 (50%)
1	GYC	B	66	1	21,22,23	3.11	7 (33%)	26,30,32	7.32	13 (50%)

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	GYC	D	66	1	-	3/10/29/30	0/2/2/2
1	GYC	C	66	1	-	2/10/29/30	0/2/2/2
1	GYC	A	66	1	-	2/10/29/30	0/2/2/2
1	GYC	B	66	1	-	2/10/29/30	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GYC	CA2-C2	9.68	1.59	1.48
1	A	66	GYC	CA2-C2	9.63	1.58	1.48
1	B	66	GYC	CA2-C2	9.59	1.58	1.48
1	A	66	GYC	C1-N2	6.53	1.41	1.32
1	B	66	GYC	C1-N2	6.52	1.41	1.32
1	C	66	GYC	C1-N2	6.51	1.41	1.32
1	C	66	GYC	CG2-CB2	4.62	1.55	1.46
1	A	66	GYC	CG2-CB2	4.59	1.55	1.46
1	B	66	GYC	CG2-CB2	4.59	1.55	1.46
1	A	66	GYC	CA2-N2	4.45	1.48	1.38
1	C	66	GYC	CA2-N2	4.44	1.48	1.38
1	B	66	GYC	CA2-N2	4.44	1.48	1.38
1	C	66	GYC	C2-N3	3.37	1.47	1.40
1	A	66	GYC	C2-N3	3.37	1.47	1.40
1	B	66	GYC	C2-N3	3.34	1.47	1.40
1	B	66	GYC	C1-N3	2.11	1.40	1.37
1	A	66	GYC	O2-C2	-2.09	1.18	1.23
1	A	66	GYC	C1-N3	2.09	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GYC	O2-C2	-2.08	1.18	1.23
1	B	66	GYC	O2-C2	-2.06	1.18	1.23
1	C	66	GYC	C1-N3	2.06	1.40	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYC	CB2-CA2-C2	26.63	154.63	122.36
1	A	66	GYC	CB2-CA2-C2	26.62	154.62	122.36
1	C	66	GYC	CB2-CA2-C2	26.60	154.60	122.36
1	B	66	GYC	CB2-CA2-N2	-20.95	100.32	128.76
1	A	66	GYC	CB2-CA2-N2	-20.94	100.33	128.76
1	C	66	GYC	CB2-CA2-N2	-20.90	100.39	128.76
1	B	66	GYC	O2-C2-CA2	-8.39	125.67	131.02
1	C	66	GYC	O2-C2-CA2	-8.36	125.69	131.02
1	A	66	GYC	O2-C2-CA2	-8.34	125.70	131.02
1	C	66	GYC	CA1-C1-N3	-6.62	116.22	124.84
1	A	66	GYC	CA1-C1-N3	-6.60	116.24	124.84
1	B	66	GYC	CA1-C1-N3	-6.59	116.25	124.84
1	C	66	GYC	C2-CA2-N2	-5.50	105.01	108.95
1	B	66	GYC	C2-CA2-N2	-5.45	105.04	108.95
1	A	66	GYC	C2-CA2-N2	-5.45	105.05	108.95
1	A	66	GYC	CG2-CB2-CA2	5.17	136.01	129.87
1	B	66	GYC	CG2-CB2-CA2	5.16	136.00	129.87
1	C	66	GYC	CG2-CB2-CA2	5.15	135.99	129.87
1	B	66	GYC	CA1-CB1-SG1	-3.73	106.42	114.40
1	C	66	GYC	CA1-CB1-SG1	-3.72	106.45	114.40
1	A	66	GYC	CA1-CB1-SG1	-3.72	106.45	114.40
1	D	66	GYC	C2-N3-C1	-3.65	106.38	108.07
1	C	66	GYC	N3-C1-N2	3.46	114.21	111.48
1	B	66	GYC	N3-C1-N2	3.46	114.21	111.48
1	A	66	GYC	N3-C1-N2	3.45	114.20	111.48
1	D	66	GYC	N3-C1-N2	3.34	114.12	111.48
1	C	66	GYC	CA1-C1-N2	3.07	129.57	123.57
1	A	66	GYC	CA1-C1-N2	3.07	129.55	123.57
1	B	66	GYC	CA1-C1-N2	3.06	129.54	123.57
1	B	66	GYC	CD1-CG2-CB2	-2.67	112.04	121.22
1	A	66	GYC	CD1-CG2-CB2	-2.67	112.06	121.22
1	C	66	GYC	CD1-CG2-CB2	-2.66	112.09	121.22
1	B	66	GYC	CA2-C2-N3	2.56	105.65	103.50
1	A	66	GYC	CA2-C2-N3	2.52	105.61	103.50
1	C	66	GYC	CA2-C2-N3	2.50	105.60	103.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GYC	CA2-N2-C1	2.24	107.56	105.80
1	A	66	GYC	CA2-N2-C1	2.20	107.52	105.80
1	B	66	GYC	CA2-N2-C1	2.19	107.51	105.80
1	D	66	GYC	O3-C3-CA3	-2.16	115.77	125.47
1	C	66	GYC	O2-C2-N3	2.11	128.72	124.31
1	A	66	GYC	O2-C2-N3	2.10	128.69	124.31
1	B	66	GYC	O2-C2-N3	2.10	128.68	124.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	GYC	C3-CA3-N3-C2
1	B	66	GYC	C3-CA3-N3-C2
1	C	66	GYC	C3-CA3-N3-C2
1	D	66	GYC	C3-CA3-N3-C1
1	A	66	GYC	C3-CA3-N3-C1
1	B	66	GYC	C3-CA3-N3-C1
1	C	66	GYC	C3-CA3-N3-C1
1	D	66	GYC	C3-CA3-N3-C2
1	D	66	GYC	N1-CA1-CB1-SG1

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	66	GYC	2	0
1	C	66	GYC	3	0
1	A	66	GYC	3	0
1	B	66	GYC	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
2	PEG	A	301	-	6,6,6	0.12	0	5,5,5	0.10	0

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	PEG	A	301	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	213/226 (94%)	0.81	14 (6%) 26 31	45, 60, 80, 93	0
1	B	216/226 (95%)	1.16	28 (12%) 9 11	48, 72, 90, 104	0
1	C	212/226 (93%)	0.97	25 (11%) 10 12	47, 63, 89, 112	0
1	D	184/226 (81%)	2.12	88 (47%) 0 1	48, 85, 121, 134	0
All	All	825/904 (91%)	1.23	155 (18%) 4 6	45, 68, 109, 134	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	MET	6.7
1	D	70	VAL	6.2
1	D	9	PRO	6.0
1	D	38	GLU	6.0
1	D	74	TYR	5.8
1	D	10	ASP	5.7
1	D	69	ARG	5.4
1	D	86	PHE	5.3
1	D	32	GLY	5.2
1	D	11	MET	5.1
1	D	37	PHE	5.0
1	D	63	ALA	4.8
1	D	78	ILE	4.8
1	D	79	VAL	4.8
1	D	80	ASP	4.7
1	D	159	ASP	4.6
1	D	212	LEU	4.6
1	D	71	PHE	4.4
1	D	85	SER	4.2
1	B	7	ILE	4.1
1	D	180	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	194	VAL	4.0
1	D	156	LEU	4.0
1	C	191	TYR	4.0
1	D	220	SER	4.0
1	D	192	HIS	4.0
1	B	185	VAL	4.0
1	D	73	LYS	4.0
1	D	117	TYR	3.9
1	D	45	LEU	3.9
1	D	119	TYR	3.9
1	D	68	ASN	3.9
1	D	33	LEU	3.9
1	D	112	LEU	3.7
1	D	151	VAL	3.7
1	D	142	TRP	3.7
1	D	87	PRO	3.7
1	D	14	LYS	3.6
1	D	149	LEU	3.6
1	D	196	HIS	3.6
1	D	162	TYR	3.5
1	C	155	VAL	3.5
1	D	13	ILE	3.5
1	A	86	PHE	3.4
1	D	77	ASN	3.4
1	B	6	VAL	3.4
1	D	84	GLN	3.3
1	C	78	ILE	3.3
1	D	183	LYS	3.3
1	D	90	TYR	3.3
1	D	118	ILE	3.2
1	D	36	PRO	3.2
1	D	39	GLY	3.2
1	D	35	LYS	3.2
1	D	44	ASP	3.2
1	B	219	HIS	3.2
1	D	40	LYS	3.1
1	D	181	LYS	3.1
1	B	110	ILE	3.1
1	D	218	ALA	3.1
1	D	15	LEU	3.1
1	A	39	GLY	3.1
1	D	215	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	188	LEU	3.0
1	D	195	VAL	3.0
1	D	76	GLU	3.0
1	D	147	GLU	3.0
1	B	11	MET	3.0
1	D	43	MET	2.9
1	D	113	ASP	2.9
1	A	71	PHE	2.9
1	A	6	VAL	2.9
1	B	222	LEU	2.9
1	C	21	VAL	2.9
1	D	216	ALA	2.9
1	D	161	ASN	2.9
1	B	103	ILE	2.8
1	D	157	LYS	2.8
1	D	219	HIS	2.8
1	C	190	ASP	2.8
1	D	193	ASP	2.8
1	A	221	GLY	2.8
1	A	146	THR	2.8
1	A	115	ASP	2.8
1	D	121	ILE	2.7
1	A	10	ASP	2.7
1	D	158	SER	2.7
1	B	24	HIS	2.7
1	B	188	LEU	2.7
1	C	168	GLY	2.7
1	B	215	HIS	2.7
1	C	81	TYR	2.6
1	B	70	VAL	2.6
1	B	151	VAL	2.6
1	B	87	PRO	2.6
1	B	33	LEU	2.6
1	B	74	TYR	2.6
1	D	75	PRO	2.6
1	C	220	SER	2.6
1	C	6	VAL	2.6
1	B	71	PHE	2.6
1	D	42	SER	2.6
1	D	214	GLU	2.6
1	A	145	SER	2.5
1	B	169	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	153	ASP	2.5
1	D	111	THR	2.5
1	B	223	PRO	2.4
1	D	201	LYS	2.4
1	D	64	PHE	2.4
1	D	110	ILE	2.4
1	D	198	ILE	2.4
1	D	200	ILE	2.4
1	A	114	GLY	2.4
1	C	76	GLU	2.4
1	C	154	GLY	2.4
1	D	88	GLU	2.4
1	C	218	ALA	2.4
1	D	182	ALA	2.4
1	C	189	PRO	2.4
1	D	105	ILE	2.4
1	D	211	ASN	2.3
1	B	213	HIS	2.3
1	D	107	THR	2.3
1	D	95	SER	2.3
1	C	142	TRP	2.3
1	C	7	ILE	2.3
1	B	194	VAL	2.2
1	D	197	HIS	2.2
1	A	7	ILE	2.2
1	D	179	THR	2.2
1	B	216	ALA	2.2
1	D	210	VAL	2.2
1	C	82	PHE	2.2
1	D	41	GLN	2.2
1	A	212	LEU	2.2
1	A	197	HIS	2.1
1	D	169	GLY	2.1
1	B	149	LEU	2.1
1	C	105	ILE	2.1
1	D	12	LYS	2.1
1	B	218	ALA	2.1
1	C	197	HIS	2.1
1	B	90	TYR	2.1
1	B	150	TYR	2.1
1	D	92	TRP	2.1
1	D	34	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	195	VAL	2.1
1	A	33	LEU	2.1
1	C	169	GLY	2.1
1	D	120	GLU	2.1
1	B	186	VAL	2.1
1	C	187	GLN	2.1
1	B	195	VAL	2.0
1	C	71	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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(Å ²)	Q<0.9
1	GYC	B	66	21/22	0.84	0.18	44,51,65,70	0
1	GYC	C	66	21/22	0.87	0.15	44,51,65,70	0
1	GYC	A	66	21/22	0.89	0.16	44,51,65,70	0
1	GYC	D	66	21/22	0.89	0.17	75,81,86,98	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(Å ²)	Q<0.9
2	PEG	A	301	7/7	0.90	0.10	56,68,72,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.