



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:08 PM UTC

PDB ID : 7PD0 / pdb_00007pd0
Title : Functional and structural characterization of redox sensitive superfolder green fluorescent protein and variants
Authors : Fritz-Wolf, K.; Heimsch, K.C.; Schuh, A.K.; Becker, K.
Deposited on : 2021-08-04
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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

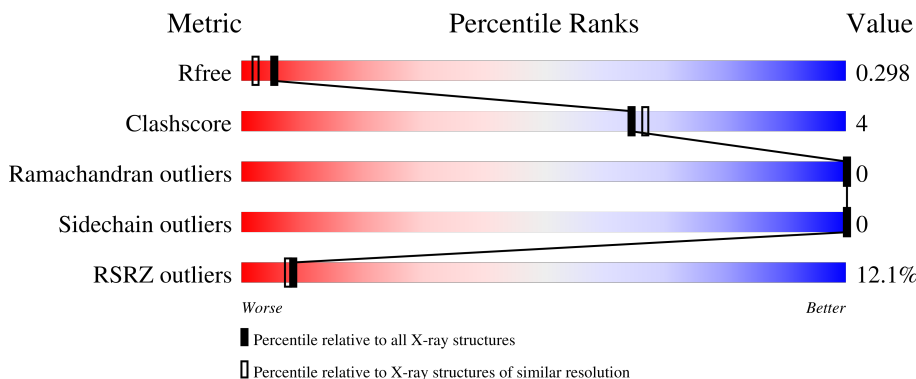
1 Overall quality at a glance

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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	236	10% 88% 9% .
1	B	236	14% 88% 8% .
1	C	236	12% 89% 10%
1	D	236	11% 89% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8017 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	1	0
			1822	1153	314	348	7			
1	B	228	Total	C	N	O	S	0	1	0
			1823	1156	313	348	6			
1	C	235	Total	C	N	O	S	0	1	0
			1878	1190	322	359	7			
1	D	236	Total	C	N	O	S	0	1	0
			1888	1198	324	359	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	MET	engineered mutation	UNP P42212
A	30	ARG	SER	engineered mutation	UNP P42212
A	48	SER	CYS	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	105	THR	ASN	engineered mutation	UNP P42212
A	145	PHE	TYR	engineered mutation	UNP P42212
A	147	CYS	SER	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	204	CYS	GLN	engineered mutation	UNP P42212
A	206	VAL	ALA	engineered mutation	UNP P42212
A	223	ARG	PHE	engineered mutation	UNP P42212
B	1	VAL	MET	engineered mutation	UNP P42212
B	30	ARG	SER	engineered mutation	UNP P42212
B	48	SER	CYS	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

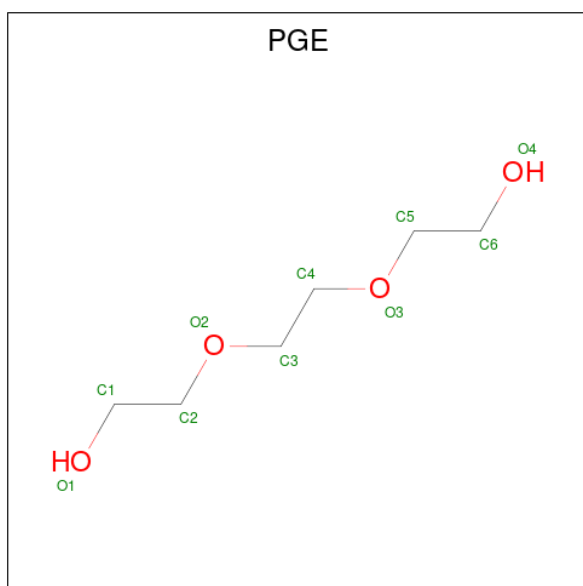
Chain	Residue	Modelled	Actual	Comment	Reference
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	105	THR	ASN	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	147	CYS	SER	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	204	CYS	GLN	engineered mutation	UNP P42212
B	206	VAL	ALA	engineered mutation	UNP P42212
B	223	ARG	PHE	engineered mutation	UNP P42212
C	1	VAL	MET	engineered mutation	UNP P42212
C	30	ARG	SER	engineered mutation	UNP P42212
C	48	SER	CYS	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	99	SER	PHE	engineered mutation	UNP P42212
C	105	THR	ASN	engineered mutation	UNP P42212
C	145	PHE	TYR	engineered mutation	UNP P42212
C	147	CYS	SER	engineered mutation	UNP P42212
C	153	THR	MET	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	171	VAL	ILE	engineered mutation	UNP P42212
C	204	CYS	GLN	engineered mutation	UNP P42212
C	206	VAL	ALA	engineered mutation	UNP P42212
C	223	ARG	PHE	engineered mutation	UNP P42212
D	1	VAL	MET	engineered mutation	UNP P42212
D	30	ARG	SER	engineered mutation	UNP P42212
D	48	SER	CYS	engineered mutation	UNP P42212
D	64	LEU	PHE	engineered mutation	UNP P42212
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212
D	99	SER	PHE	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

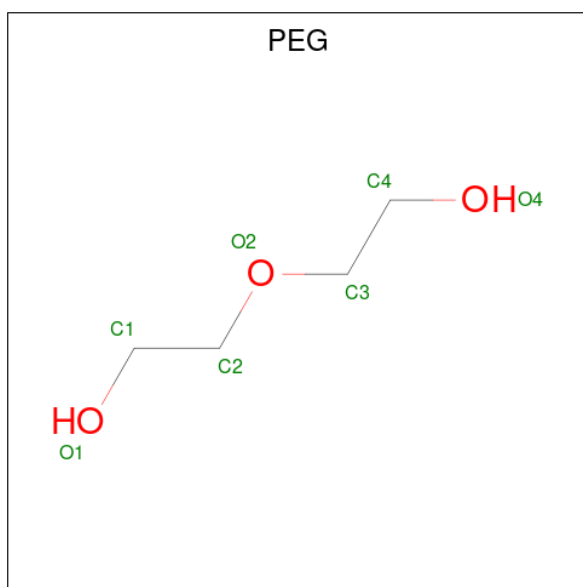
Chain	Residue	Modelled	Actual	Comment	Reference
D	105	THR	ASN	engineered mutation	UNP P42212
D	145	PHE	TYR	engineered mutation	UNP P42212
D	147	CYS	SER	engineered mutation	UNP P42212
D	153	THR	MET	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	171	VAL	ILE	engineered mutation	UNP P42212
D	204	CYS	GLN	engineered mutation	UNP P42212
D	206	VAL	ALA	engineered mutation	UNP P42212
D	223	ARG	PHE	engineered mutation	UNP P42212

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



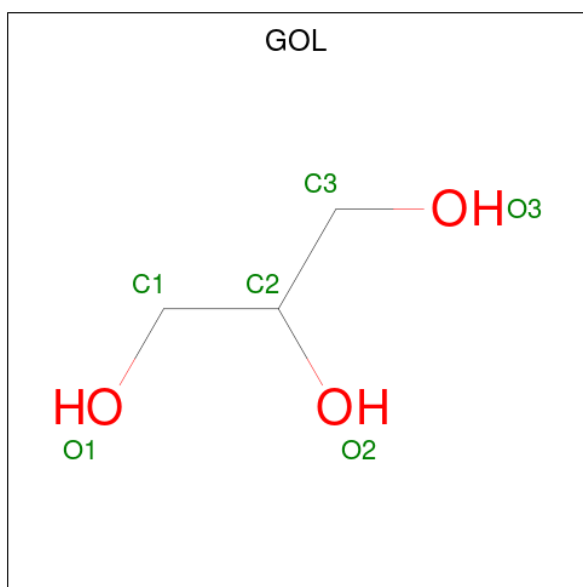
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

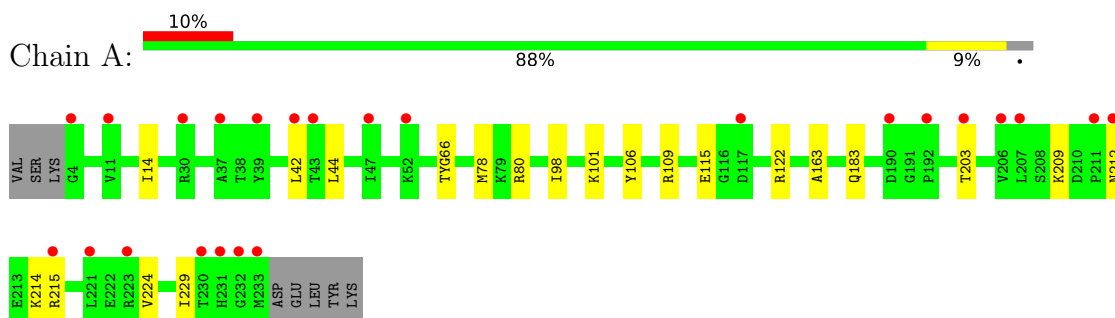
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	107	Total	O	0	0
			107	107		
5	B	110	Total	O	0	0
			110	110		
5	C	148	Total	O	0	0
			148	148		
5	D	156	Total	O	0	0
			156	156		

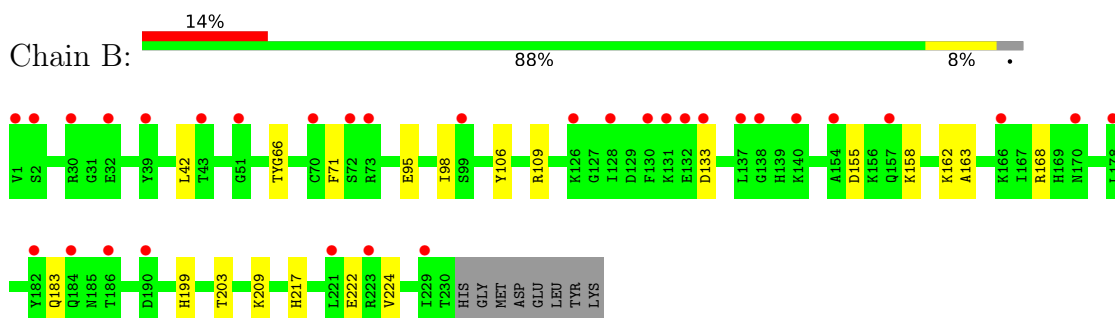
3 Residue-property plots [i](#)

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.

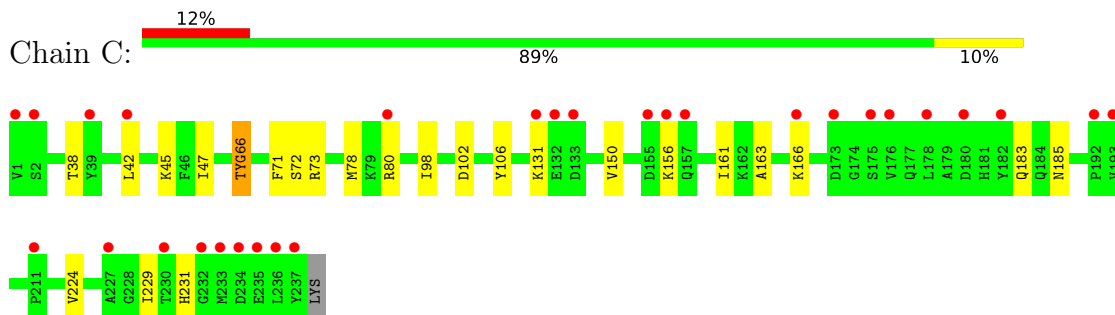
- Molecule 1: Green fluorescent protein



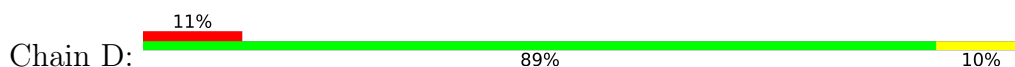
- Molecule 1: Green fluorescent protein

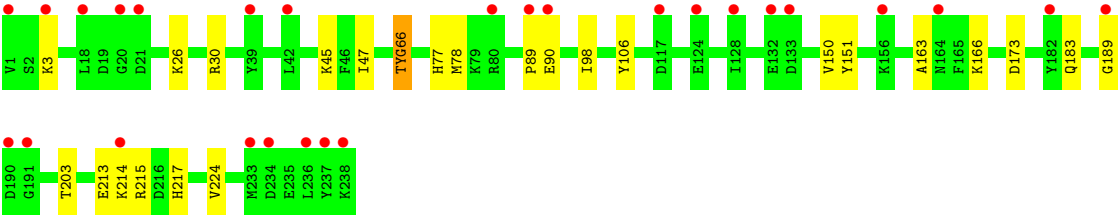


- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.85Å 51.29Å 101.46Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	47.92 – 2.00 47.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.92-2.00) 94.8 (47.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.250 , 0.298 0.250 , 0.298	Depositor DCC
R_{free} test set	4596 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.44$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8017	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 58.86 % 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 1.9225e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.10	0/1842	0.28	0/2489
1	B	0.12	0/1842	0.29	0/2489
1	C	0.12	0/1899	0.30	0/2566
1	D	0.12	0/1909	0.32	0/2578
All	All	0.11	0/7492	0.30	0/10122

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	1778	12	1
1	B	1823	0	1793	12	1
1	C	1878	0	1836	18	0
1	D	1888	0	1853	17	0
2	A	20	0	28	1	0
2	C	10	0	14	1	0
3	A	7	0	10	1	0
3	B	14	0	20	0	0
3	C	21	0	30	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	10	0	0
4	D	6	0	8	0	0
5	A	107	0	0	1	0
5	B	110	0	0	2	0
5	C	148	0	0	4	0
5	D	156	0	0	3	0
All	All	8017	0	7380	58	1

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 4.

All (58) 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:163:ALA:HB3	1:C:183:GLN:HB3	1.72	0.71
1:B:163:ALA:HB3	1:B:183:GLN:HB3	1.77	0.67
1:C:45:LYS:HE2	1:C:47:ILE:HD11	1.76	0.67
1:A:215:ARG:NH1	5:A:401:HOH:O	2.27	0.66
1:D:163:ALA:HB3	1:D:183:GLN:HB3	1.78	0.65
1:D:98:ILE:HB	1:D:106:TYR:HB2	1.79	0.64
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.80	0.63
1:B:203:THR:HG23	1:B:224:VAL:HG22	1.82	0.61
1:B:168:ARG:NH1	5:B:401:HOH:O	2.34	0.61
1:A:203:THR:HG23	1:A:224:VAL:HG22	1.83	0.61
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.83	0.60
1:C:73:ARG:NH2	5:C:506:HOH:O	2.35	0.60
1:A:101:LYS:NZ	1:D:173:ASP:OD2	2.29	0.59
1:B:98:ILE:HB	1:B:106:TYR:HB2	1.84	0.58
1:C:98:ILE:HB	1:C:106:TYR:HB2	1.85	0.58
1:D:26:LYS:NZ	5:D:410:HOH:O	2.37	0.57
1:C:80:ARG:NH1	5:C:504:HOH:O	2.38	0.56
1:D:3:LYS:NZ	1:D:89:PRO:HD2	2.19	0.56
1:D:203:THR:HG23	1:D:224:VAL:HG22	1.87	0.55
1:C:42:LEU:HD11	1:C:71:PHE:CB	2.37	0.55
1:C:80:ARG:CZ	1:C:80:ARG:HB2	2.37	0.55
1:C:73:ARG:NH1	5:C:510:HOH:O	2.39	0.54
1:A:115:GLU:OE2	1:A:122:ARG:NH1	2.37	0.53
1:C:72:SER:HA	1:C:224:VAL:HG13	1.91	0.53
1:B:155:ASP:OD2	1:B:162:LYS:NZ	2.42	0.53
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.74	0.52
1:D:77:HIS:CE1	1:D:78:MET:HG3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42[B]:LEU:HD21	1:B:71:PHE:CG	2.47	0.50
1:A:209:LYS:HB2	2:A:301:PGE:H5	1.95	0.49
1:C:42:LEU:HD11	1:C:71:PHE:HB2	1.93	0.49
1:A:42:LEU:HD13	1:A:44:LEU:HD12	1.94	0.49
1:D:66:CRO:HD2	1:D:150:VAL:HG21	1.95	0.48
1:A:78:MET:HG2	1:A:229:ILE:HB	1.94	0.48
1:C:102:ASP:O	1:C:131:LYS:HE2	2.13	0.48
1:B:42[A]:LEU:HG	1:B:222:GLU:HB3	1.94	0.48
1:A:14:ILE:HB	1:A:44:LEU:HD21	1.94	0.47
1:C:166:LYS:NZ	5:C:518:HOH:O	2.49	0.46
1:B:95:GLU:HG2	1:B:109:ARG:HG3	1.97	0.46
1:B:209:LYS:NZ	1:B:217:HIS:O	2.41	0.46
1:C:38:THR:HA	3:C:404:PEG:H31	1.97	0.45
1:D:3:LYS:HZ1	1:D:89:PRO:HD2	1.81	0.44
1:D:90:GLU:HG3	1:D:189:GLY:HA3	1.99	0.43
1:B:199:HIS:HA	1:D:151:TYR:OH	2.19	0.43
1:C:66:CRO:HD2	1:C:150:VAL:HG21	2.01	0.43
1:C:161:ILE:HG13	1:C:185:ASN:HB2	2.01	0.43
1:D:45:LYS:HE2	1:D:47:ILE:HD11	2.00	0.43
1:B:158:LYS:NZ	5:B:404:HOH:O	2.38	0.43
1:D:214:LYS:HE2	1:D:214:LYS:HB2	1.81	0.42
1:D:30:ARG:NH1	5:D:413:HOH:O	2.52	0.42
1:D:166:LYS:NZ	5:D:417:HOH:O	2.46	0.42
1:A:212:ASN:O	1:A:214:LYS:NZ	2.46	0.41
1:D:213:GLU:HG2	1:D:217:HIS:CG	2.55	0.41
1:D:213:GLU:OE2	1:D:215:ARG:NE	2.44	0.41
1:B:42[B]:LEU:HD21	1:B:71:PHE:CB	2.51	0.41
1:C:78:MET:HE3	1:C:229:ILE:HG13	2.02	0.41
1:C:231:HIS:NE2	2:C:401:PGE:O4	2.50	0.41
1:C:156:LYS:HE2	1:C:156:LYS:HB2	1.81	0.41
3:A:302:PEG:H11	3:A:302:PEG:H32	1.96	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:NH1	1:B:133:ASP:OD1[1_554]	1.65	0.55

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	224/236 (95%)	220 (98%)	4 (2%)	0	100	100
1	B	224/236 (95%)	221 (99%)	3 (1%)	0	100	100
1	C	231/236 (98%)	227 (98%)	4 (2%)	0	100	100
1	D	232/236 (98%)	227 (98%)	5 (2%)	0	100	100
All	All	911/944 (96%)	895 (98%)	16 (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	199/206 (97%)	199 (100%)	0	100	100
1	B	200/206 (97%)	200 (100%)	0	100	100
1	C	205/206 (100%)	205 (100%)	0	100	100
1	D	206/206 (100%)	206 (100%)	0	100	100
All	All	810/824 (98%)	810 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	C	135	ASN
1	C	146	ASN
1	C	212	ASN
1	D	212	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	CRO	A	66	1	22,23,24	2.99	6 (27%)	30,32,34	2.32	6 (20%)
1	CRO	B	66	1	22,23,24	3.02	6 (27%)	30,32,34	2.42	6 (20%)
1	CRO	D	66	1	22,23,24	2.99	6 (27%)	30,32,34	2.34	6 (20%)
1	CRO	C	66	1	22,23,24	3.00	6 (27%)	30,32,34	2.34	6 (20%)

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	CRO	A	66	1	-	2/12/31/32	0/2/2/2
1	CRO	B	66	1	-	3/12/31/32	0/2/2/2
1	CRO	D	66	1	-	3/12/31/32	0/2/2/2
1	CRO	C	66	1	-	3/12/31/32	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	C1-N2	7.17	1.42	1.32
1	D	66	CRO	C1-N2	7.09	1.42	1.32
1	C	66	CRO	C1-N2	7.04	1.42	1.32
1	A	66	CRO	C1-N2	7.04	1.42	1.32
1	B	66	CRO	CG2-CB2	6.14	1.58	1.46
1	C	66	CRO	CA2-C2	6.12	1.55	1.48
1	C	66	CRO	CG2-CB2	6.12	1.58	1.46
1	D	66	CRO	CA2-C2	6.11	1.55	1.48
1	A	66	CRO	CG2-CB2	6.09	1.58	1.46
1	B	66	CRO	CA2-C2	6.08	1.55	1.48
1	D	66	CRO	CG2-CB2	6.07	1.58	1.46
1	A	66	CRO	CA2-C2	6.04	1.55	1.48
1	C	66	CRO	C1-N3	6.02	1.47	1.37
1	B	66	CRO	C1-N3	6.02	1.47	1.37
1	D	66	CRO	C1-N3	5.98	1.47	1.37
1	A	66	CRO	C1-N3	5.97	1.47	1.37
1	C	66	CRO	C2-N3	3.98	1.49	1.40
1	B	66	CRO	C2-N3	3.95	1.49	1.40
1	D	66	CRO	C2-N3	3.91	1.49	1.40
1	A	66	CRO	C2-N3	3.91	1.49	1.40
1	C	66	CRO	CA2-N2	2.64	1.44	1.38
1	A	66	CRO	CA2-N2	2.63	1.44	1.38
1	B	66	CRO	CA2-N2	2.61	1.44	1.38
1	D	66	CRO	CA2-N2	2.58	1.44	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	O2-C2-CA2	-7.99	125.92	131.02
1	D	66	CRO	O2-C2-CA2	-7.91	125.97	131.02
1	C	66	CRO	O2-C2-CA2	-7.82	126.03	131.02
1	A	66	CRO	O2-C2-CA2	-7.59	126.17	131.02
1	B	66	CRO	C2-N3-C1	-5.93	105.32	108.07
1	A	66	CRO	C2-N3-C1	-5.59	105.48	108.07
1	C	66	CRO	C2-N3-C1	-5.58	105.48	108.07
1	D	66	CRO	C2-N3-C1	-5.41	105.56	108.07
1	B	66	CRO	CA2-C2-N3	4.22	107.05	103.50
1	B	66	CRO	CA2-N2-C1	4.06	108.98	105.80
1	C	66	CRO	CG2-CB2-CA2	-3.97	125.14	129.87
1	A	66	CRO	CA2-C2-N3	3.96	106.82	103.50
1	D	66	CRO	CA2-N2-C1	3.91	108.86	105.80
1	A	66	CRO	CA2-N2-C1	3.91	108.86	105.80
1	D	66	CRO	CG2-CB2-CA2	-3.86	125.27	129.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	CG2-CB2-CA2	-3.85	125.29	129.87
1	D	66	CRO	CA2-C2-N3	3.84	106.72	103.50
1	C	66	CRO	CA2-C2-N3	3.80	106.69	103.50
1	C	66	CRO	CA2-N2-C1	3.79	108.76	105.80
1	A	66	CRO	CG2-CB2-CA2	-3.74	125.42	129.87
1	B	66	CRO	C2-CA2-N2	-3.10	106.73	108.95
1	A	66	CRO	C2-CA2-N2	-2.87	106.90	108.95
1	D	66	CRO	C2-CA2-N2	-2.76	106.98	108.95
1	C	66	CRO	C2-CA2-N2	-2.66	107.04	108.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	C2-CA2-CB2-CG2
1	D	66	CRO	C2-CA2-CB2-CG2
1	C	66	CRO	N2-CA2-CB2-CG2
1	D	66	CRO	N2-CA2-CB2-CG2
1	A	66	CRO	N2-CA2-CB2-CG2
1	B	66	CRO	N2-CA2-CB2-CG2
1	C	66	CRO	C3-CA3-N3-C2
1	D	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	C2-CA2-CB2-CG2
1	A	66	CRO	C2-CA2-CB2-CG2
1	B	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands 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	$\# Z > 2$
2	PGE	A	301	-	9,9,9	0.78	0	8,8,8	0.26	0
3	PEG	B	302	-	6,6,6	0.75	0	5,5,5	0.29	0
2	PGE	C	401	-	9,9,9	0.77	0	8,8,8	0.25	0
4	GOL	D	302	-	5,5,5	0.92	0	5,5,5	1.08	0
3	PEG	A	302	-	6,6,6	0.75	0	5,5,5	0.31	0
2	PGE	A	303	-	9,9,9	0.77	0	8,8,8	0.28	0
3	PEG	C	402	-	6,6,6	0.75	0	5,5,5	0.27	0
3	PEG	D	301	-	6,6,6	0.75	0	5,5,5	0.29	0
3	PEG	C	403	-	6,6,6	0.76	0	5,5,5	0.28	0
3	PEG	C	404	-	6,6,6	0.77	0	5,5,5	0.30	0
3	PEG	B	301	-	6,6,6	0.75	0	5,5,5	0.30	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	PGE	A	301	-	-	1/7/7/7	-
3	PEG	B	302	-	-	0/4/4/4	-
2	PGE	C	401	-	-	3/7/7/7	-
4	GOL	D	302	-	-	2/4/4/4	-
3	PEG	A	302	-	-	3/4/4/4	-
2	PGE	A	303	-	-	5/7/7/7	-
3	PEG	C	402	-	-	1/4/4/4	-
3	PEG	D	301	-	-	1/4/4/4	-
3	PEG	C	403	-	-	2/4/4/4	-
3	PEG	C	404	-	-	3/4/4/4	-
3	PEG	B	301	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	302	GOL	C1-C2-C3-O3
4	D	302	GOL	O2-C2-C3-O3
2	A	303	PGE	O3-C5-C6-O4
3	C	403	PEG	O1-C1-C2-O2
3	B	301	PEG	O1-C1-C2-O2
3	A	302	PEG	C1-C2-O2-C3
2	C	401	PGE	C1-C2-O2-C3
3	C	404	PEG	C4-C3-O2-C2
2	A	301	PGE	C4-C3-O2-C2
2	A	303	PGE	O2-C3-C4-O3
3	A	302	PEG	O1-C1-C2-O2
3	C	403	PEG	C4-C3-O2-C2
2	A	303	PGE	C1-C2-O2-C3
3	C	404	PEG	O1-C1-C2-O2
3	C	402	PEG	C1-C2-O2-C3
3	D	301	PEG	O2-C3-C4-O4
2	C	401	PGE	O2-C3-C4-O3
2	C	401	PGE	C6-C5-O3-C4
3	A	302	PEG	C4-C3-O2-C2
2	A	303	PGE	O1-C1-C2-O2
3	C	404	PEG	O2-C3-C4-O4
2	A	303	PGE	C6-C5-O3-C4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PGE	1	0
2	C	401	PGE	1	0
3	A	302	PEG	1	0
3	C	404	PEG	1	0

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, 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	227/236 (96%)	1.11	24 (10%)	11 10	19, 30, 46, 104	1 (0%)
1	B	227/236 (96%)	1.14	32 (14%)	6 5	19, 31, 48, 62	1 (0%)
1	C	234/236 (99%)	1.10	29 (12%)	8 7	15, 27, 48, 60	1 (0%)
1	D	235/236 (99%)	1.02	27 (11%)	9 8	15, 26, 45, 67	1 (0%)
All	All	923/944 (97%)	1.09	112 (12%)	8 8	15, 29, 48, 104	4 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	237	TYR	6.8
1	A	231	HIS	6.7
1	C	233	MET	5.4
1	A	233	MET	5.3
1	C	175	SER	5.0
1	D	1	VAL	4.9
1	D	238	LYS	4.6
1	A	232	GLY	4.3
1	D	164	ASN	4.2
1	B	30	ARG	4.1
1	A	230	THR	4.1
1	B	43	THR	4.1
1	B	1	VAL	4.0
1	C	1	VAL	4.0
1	A	39	TYR	3.9
1	D	237	TYR	3.9
1	C	2	SER	3.9
1	D	124	GLU	3.7
1	D	89	PRO	3.7
1	D	214	LYS	3.5
1	C	80	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	4	GLY	3.4
1	C	132	GLU	3.4
1	B	223	ARG	3.4
1	B	2	SER	3.3
1	A	52	LYS	3.2
1	D	39	TYR	3.2
1	C	133	ASP	3.2
1	C	178	LEU	3.1
1	C	39	TYR	3.1
1	C	230	THR	3.1
1	D	90	GLU	3.1
1	C	157	GLN	3.1
1	A	221	LEU	3.1
1	A	43	THR	3.0
1	B	70	CYS	3.0
1	D	191	GLY	3.0
1	D	3	LYS	3.0
1	A	30	ARG	2.9
1	C	42	LEU	2.9
1	B	39	TYR	2.9
1	C	156	LYS	2.9
1	B	140	LYS	2.7
1	A	223	ARG	2.7
1	C	176	VAL	2.7
1	C	234	ASP	2.7
1	B	132	GLU	2.6
1	B	178	LEU	2.6
1	B	186	THR	2.6
1	D	236	LEU	2.6
1	A	117	ASP	2.6
1	D	133	ASP	2.6
1	D	182	TYR	2.6
1	A	211	PRO	2.6
1	B	128	ILE	2.6
1	C	131	LYS	2.6
1	A	11	VAL	2.5
1	A	47	ILE	2.5
1	C	193	VAL	2.5
1	D	42	LEU	2.5
1	C	180	ASP	2.5
1	C	173	ASP	2.4
1	B	154	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	131	LYS	2.4
1	D	132	GLU	2.4
1	A	206	VAL	2.4
1	B	133	ASP	2.4
1	C	155	ASP	2.4
1	C	236	LEU	2.4
1	B	126	LYS	2.4
1	D	117	ASP	2.3
1	D	80	ARG	2.3
1	D	156	LYS	2.3
1	B	229	ILE	2.3
1	A	212	ASN	2.3
1	B	138	GLY	2.3
1	B	221	LEU	2.3
1	D	234	ASP	2.3
1	D	189	GLY	2.3
1	D	21	ASP	2.2
1	A	207	LEU	2.2
1	B	137	LEU	2.2
1	D	18[A]	LEU	2.2
1	C	235	GLU	2.2
1	C	192	PRO	2.2
1	D	128	ILE	2.2
1	A	37	ALA	2.2
1	C	227	ALA	2.2
1	A	215	ARG	2.2
1	B	190	ASP	2.2
1	D	190	ASP	2.2
1	B	32	GLU	2.2
1	B	51	GLY	2.2
1	A	42	LEU	2.2
1	C	182	TYR	2.2
1	A	192	PRO	2.1
1	B	72	SER	2.1
1	B	99	SER	2.1
1	D	233	MET	2.1
1	C	211	PRO	2.1
1	B	130	PHE	2.1
1	B	170	ASN	2.1
1	C	232	GLY	2.1
1	B	166	LYS	2.1
1	A	190	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	157	GLN	2.1
1	A	203	THR	2.1
1	B	73	ARG	2.1
1	C	166	LYS	2.0
1	D	20	GLY	2.0
1	B	184	GLN	2.0
1	B	182	TYR	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	CRO	C	66	22/23	0.86	0.13	17,19,22,23	0
1	CRO	A	66	22/23	0.87	0.11	18,23,27,29	0
1	CRO	B	66	22/23	0.88	0.12	21,24,27,28	0
1	CRO	D	66	22/23	0.90	0.11	16,20,24,28	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
3	PEG	B	301	7/7	0.49	0.27	61,61,63,64	0
3	PEG	D	301	7/7	0.56	0.26	57,62,65,65	0
3	PEG	C	404	7/7	0.61	0.23	29,40,43,45	0
2	PGE	A	301	10/10	0.61	0.25	44,52,55,58	0
3	PEG	A	302	7/7	0.65	0.24	50,56,58,61	0
2	PGE	A	303	10/10	0.69	0.19	58,62,62,63	0
3	PEG	C	403	7/7	0.70	0.23	56,59,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PGE	C	401	10/10	0.71	0.25	60,64,65,66	0
4	GOL	D	302	6/6	0.71	0.27	57,59,59,59	0
3	PEG	B	302	7/7	0.78	0.19	48,52,54,55	0
3	PEG	C	402	7/7	0.80	0.16	39,45,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.