



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 6D01 / pdb_00006d01
Title : Crystal structure of 1210 Fab in complex with circumsporozoite protein NANP5
Authors : Scally, S.W.; Bosch, A.; Imkeller, K.; Wardemann, H.; Julien, J.P.
Deposited on : 2018-04-09
Resolution : 3.20 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

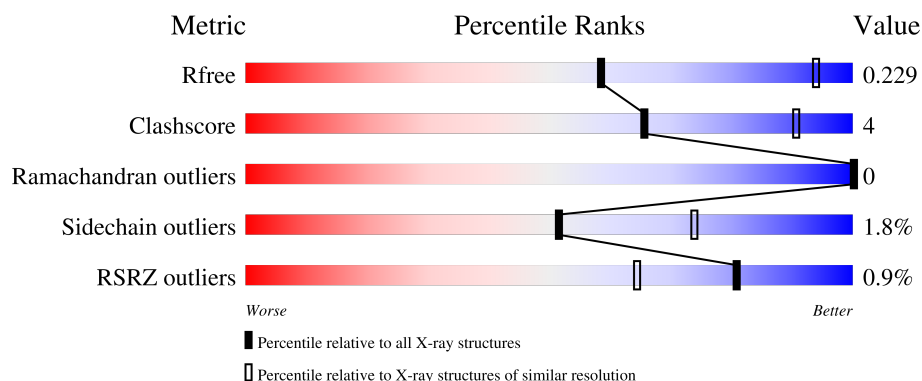
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	% 85% 13% .
1	C	226	85% 12% .
1	E	226	% 84% 14% .
1	G	226	% 85% 12% .
2	B	213	92% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	213	 91% 7% 2%
2	F	213	 93% 6% 2%
2	H	213	 92% 8%
3	I	20	 85% 10% 10%
3	J	20	 75% 20% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	J	101	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13609 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 1210 Antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1655	1045	280	323	7			
1	C	220	Total	C	N	O	S	0	0	0
			1633	1032	274	320	7			
1	E	222	Total	C	N	O	S	0	0	0
			1652	1043	277	325	7			
1	G	219	Total	C	N	O	S	0	0	0
			1643	1037	279	320	7			

- Molecule 2 is a protein called 1210 Antibody, Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1622	1017	270	330	5			
2	D	212	Total	C	N	O	S	0	0	0
			1634	1025	272	332	5			
2	F	212	Total	C	N	O	S	0	0	0
			1630	1023	272	330	5			
2	H	213	Total	C	N	O	S	0	0	0
			1636	1025	272	333	6			

- Molecule 3 is a protein called NANP5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	19	Total	C	N	O	0	0	0
			132	76	28	28			
3	J	19	Total	C	N	O	0	0	0
			132	76	28	28			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

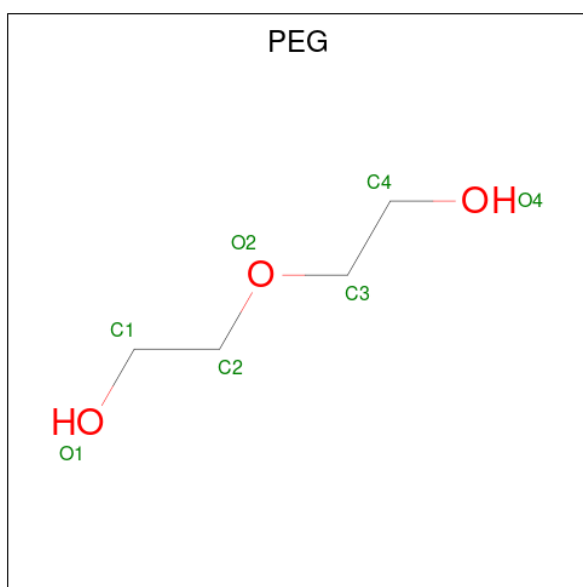
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

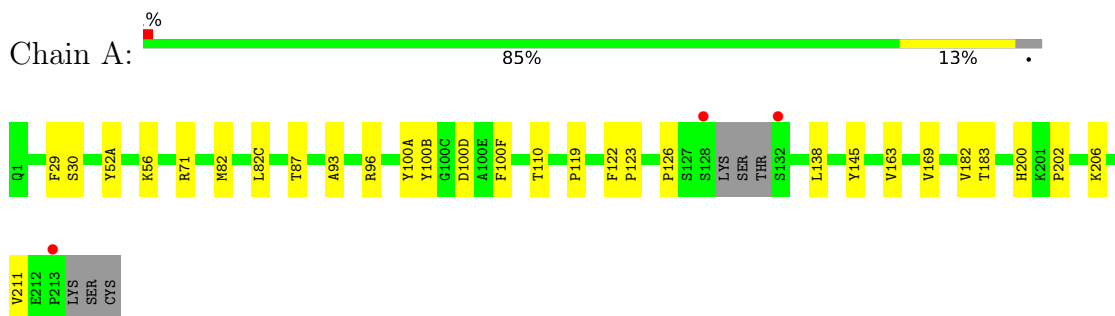


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		

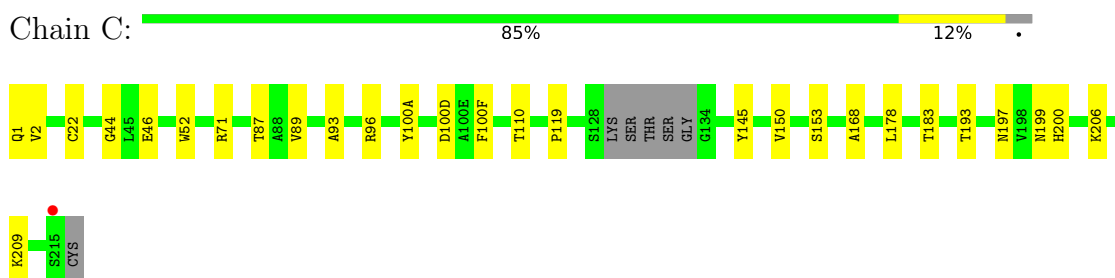
3 Residue-property plots [i](#)

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.

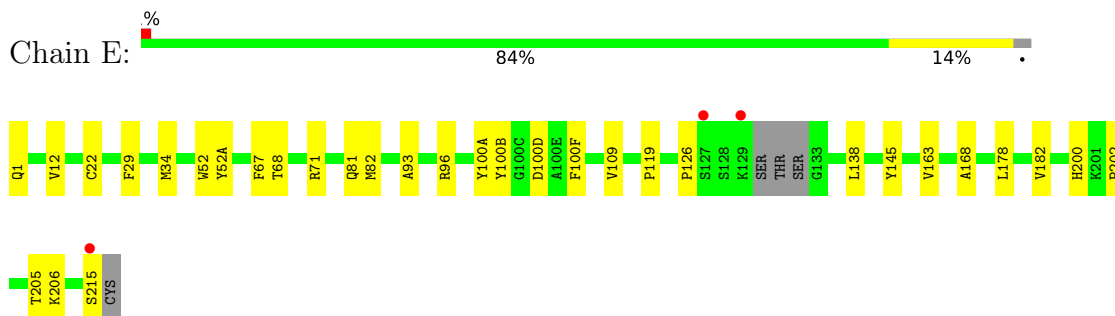
- Molecule 1: 1210 Antibody, heavy chain



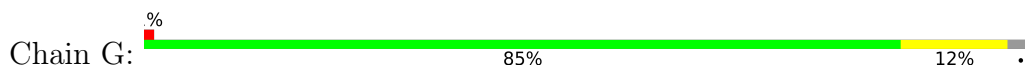
- Molecule 1: 1210 Antibody, heavy chain



- Molecule 1: 1210 Antibody, heavy chain



- Molecule 1: 1210 Antibody, heavy chain





- Molecule 2: 1210 Antibody, Light chain



- Molecule 2: 1210 Antibody, Light chain



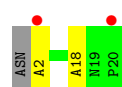
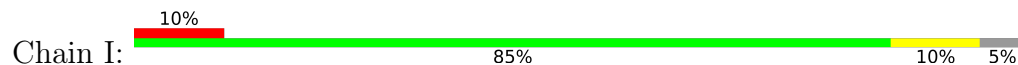
- Molecule 2: 1210 Antibody, Light chain



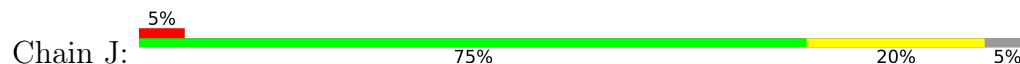
- Molecule 2: 1210 Antibody, Light chain



- Molecule 3: NANP5



- Molecule 3: NANP5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.96Å 150.86Å 134.65Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	39.87 – 3.20 39.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.87-3.20) 93.4 (39.87-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.204 , 0.227 0.206 , 0.229	Depositor DCC
R_{free} test set	2001 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13609	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.87% 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, EDO

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	0.09	0/1696	0.29	0/2311
1	C	0.10	0/1674	0.31	0/2286
1	E	0.10	0/1693	0.29	0/2310
1	G	0.10	0/1684	0.31	0/2297
2	B	0.10	0/1659	0.30	0/2261
2	D	0.14	0/1671	0.34	0/2274
2	F	0.10	0/1667	0.30	0/2269
2	H	0.10	0/1673	0.31	0/2278
3	I	0.16	0/136	0.31	0/191
3	J	0.16	0/136	0.30	0/191
All	All	0.11	0/13689	0.31	0/18668

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	1655	0	1590	17	0
1	C	1633	0	1544	14	0
1	E	1652	0	1569	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1643	0	1565	14	0
2	B	1622	0	1539	10	0
2	D	1634	0	1565	13	0
2	F	1630	0	1561	6	0
2	H	1636	0	1559	7	0
3	I	132	0	113	2	0
3	J	132	0	113	3	0
4	A	16	0	24	3	0
4	B	44	0	66	4	0
4	C	12	0	18	1	0
4	D	32	0	48	2	0
4	E	16	0	24	1	0
4	F	28	0	42	0	0
4	G	4	0	6	0	0
4	H	16	0	24	2	0
4	I	12	0	18	0	0
4	J	4	0	6	1	0
5	A	7	0	10	1	0
5	B	14	0	20	1	0
5	C	7	0	10	3	0
5	D	7	0	10	2	0
5	E	7	0	10	0	0
5	F	14	0	20	1	0
All	All	13609	0	13074	102	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 4.

All (102) 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:199:ASN:HB2	1:C:206:LYS:HZ3	1.49	0.78
2:F:39:LYS:NZ	2:F:81:ASP:OD1	2.24	0.71
1:G:52:TRP:O	1:G:71:ARG:NH1	2.25	0.68
1:G:82:MET:HE2	1:G:82(C):LEU:HD21	1.76	0.68
1:E:93:ALA:HB1	1:E:100(F):PHE:HB3	1.76	0.67
1:E:100(A):TYR:HH	3:J:2:ALA:N	1.92	0.67
1:A:56:LYS:HG2	4:A:301:EDO:H21	1.77	0.67
1:A:100(A):TYR:HH	3:I:2:ALA:N	1.94	0.66
4:A:304:EDO:H11	5:A:305:PEG:H42	1.80	0.64
5:C:304:PEG:H41	2:D:97:THR:HA	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:PRO:HB3	1:G:145:TYR:HB3	1.79	0.63
1:A:93:ALA:HB1	1:A:100(F):PHE:HB3	1.79	0.63
1:A:82:MET:HE2	1:A:82(C):LEU:HD21	1.81	0.62
1:C:46:GLU:HA	5:C:304:PEG:H42	1.82	0.62
1:E:126:PRO:HG3	1:E:138:LEU:HB3	1.82	0.61
1:G:93:ALA:HB1	1:G:100(F):PHE:HB3	1.82	0.61
2:B:42:LYS:HZ3	4:B:308:EDO:H21	1.66	0.61
1:C:93:ALA:HB1	1:C:100(F):PHE:HB3	1.81	0.60
4:D:305:EDO:H12	5:D:309:PEG:H12	1.81	0.60
1:G:87:THR:HG23	1:G:110:THR:HA	1.84	0.59
1:E:119:PRO:HB3	1:E:145:TYR:HB3	1.84	0.59
2:H:183:LYS:NZ	2:H:187:GLU:OE2	2.31	0.58
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.85	0.58
1:A:29:PHE:O	1:A:71:ARG:NH2	2.36	0.57
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.86	0.57
2:H:145:LYS:HB3	2:H:197:THR:HB	1.88	0.56
1:A:87:THR:HG23	1:A:110:THR:HA	1.88	0.55
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.88	0.55
1:A:100(B):TYR:HB2	1:C:100(A):TYR:HD1	1.72	0.55
1:C:52:TRP:O	1:C:71:ARG:NH1	2.39	0.54
1:C:87:THR:HG23	1:C:110:THR:HA	1.89	0.54
2:B:42:LYS:NZ	4:B:308:EDO:H21	2.23	0.53
5:C:304:PEG:H32	2:D:97:THR:HG22	1.91	0.53
2:D:158:ASN:OD1	2:D:158:ASN:N	2.41	0.53
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.92	0.52
1:A:52(A):TYR:HA	1:A:71:ARG:NH1	2.25	0.52
1:E:67:PHE:CE2	1:E:82:MET:HG2	2.45	0.52
2:H:158:ASN:HB2	2:H:179:LEU:HD12	1.92	0.52
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.92	0.51
5:B:313:PEG:H21	4:H:304:EDO:H22	1.92	0.50
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.94	0.50
1:G:52:TRP:HE1	4:J:101:EDO:H21	1.77	0.50
1:E:100(B):TYR:HB2	1:G:100(A):TYR:HD1	1.77	0.50
1:E:200:HIS:CD2	1:E:202:PRO:HD2	2.47	0.50
2:B:145:LYS:HB3	2:B:197:THR:HB	1.93	0.49
2:D:188:LYS:HD2	2:D:188:LYS:HA	1.52	0.49
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.94	0.49
2:D:125:LEU:O	2:D:183:LYS:HE3	2.12	0.48
1:E:96:ARG:HB3	1:E:100(D):ASP:HB3	1.96	0.48
1:C:178:LEU:HA	4:D:303:EDO:H11	1.96	0.48
1:G:32:TYR:CE1	1:G:97:ASP:HB2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:ASN:HB2	2:F:179:LEU:HD12	1.95	0.47
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.96	0.47
2:B:147:GLN:HB3	2:B:154:LEU:HD11	1.95	0.47
1:A:126:PRO:HG3	1:A:138:LEU:HD23	1.97	0.46
4:A:304:EDO:H21	2:B:94:TYR:CZ	2.50	0.46
1:C:44:GLY:HA3	4:C:303:EDO:H11	1.97	0.46
1:E:119:PRO:HD2	1:E:205:THR:HG21	1.98	0.46
1:E:68:THR:HB	1:E:81:GLN:HB3	1.97	0.46
2:D:142:ARG:HE	2:D:163:VAL:HG11	1.81	0.46
1:E:82:MET:HE1	1:E:109:VAL:HG11	1.99	0.45
1:G:200:HIS:CD2	1:G:202:PRO:HD2	2.51	0.45
1:A:96:ARG:HB3	1:A:100(D):ASP:HB3	1.98	0.45
1:C:150:VAL:HG12	1:C:200:HIS:HD2	1.82	0.45
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.52	0.45
1:E:52:TRP:O	1:E:71:ARG:NH1	2.46	0.45
1:A:123:PRO:HB3	1:A:211:VAL:HG22	1.98	0.44
1:G:34:MET:HB3	1:G:78:LEU:HD22	2.00	0.44
2:H:8:PRO:HB2	4:H:301:EDO:H11	2.00	0.44
1:G:33:GLY:HA3	3:J:8:PRO:HB2	2.00	0.44
1:G:163:VAL:HG22	1:G:182:VAL:HB	1.99	0.44
1:E:29:PHE:HE1	1:E:34:MET:HE2	1.83	0.43
2:H:120:PRO:HD3	2:H:132:VAL:HG22	1.99	0.43
1:E:168:ALA:HA	1:E:178:LEU:HB3	2.00	0.43
2:D:24:ARG:NE	2:D:70:GLU:OE2	2.46	0.43
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.53	0.43
1:E:52(A):TYR:HA	1:E:71:ARG:NH1	2.34	0.43
4:B:303:EDO:H12	2:D:50:LYS:NZ	2.34	0.42
1:G:52(A):TYR:HA	1:G:71:ARG:NH1	2.34	0.42
1:E:163:VAL:HG22	1:E:182:VAL:HB	2.00	0.42
1:A:52(A):TYR:CD1	3:I:18:ALA:HB2	2.54	0.42
2:F:107:LYS:HA	2:F:140:TYR:OH	2.20	0.42
1:C:150:VAL:HG12	1:C:200:HIS:CD2	2.55	0.41
5:D:309:PEG:O4	5:F:309:PEG:O4	2.31	0.41
2:B:42:LYS:HE3	4:B:307:EDO:H22	2.01	0.41
2:D:39:LYS:HG2	2:D:84:ALA:HB2	2.02	0.41
2:D:105:GLU:HG2	2:D:106:ILE:N	2.36	0.41
1:A:163:VAL:HG22	1:A:182:VAL:HB	2.02	0.41
1:E:96:ARG:HH22	4:E:303:EDO:H11	1.86	0.41
2:H:146:VAL:HG22	2:H:196:VAL:HG22	2.02	0.41
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.56	0.41
1:E:206:LYS:HE2	1:E:206:LYS:HB3	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HA	1:A:123:PRO:HD3	1.91	0.40
1:A:206:LYS:HE3	1:A:206:LYS:HB2	1.89	0.40
2:D:183:LYS:HE2	2:D:183:LYS:HB2	1.80	0.40
1:G:94:ARG:CZ	1:G:102:ILE:HD12	2.51	0.40
1:C:96:ARG:HB3	1:C:100(D):ASP:HB3	2.02	0.40
1:C:153:SER:O	1:C:197:ASN:N	2.46	0.40
2:F:33:LEU:HD22	2:F:71:PHE:CG	2.56	0.40
3:J:18:ALA:O	3:J:20:PRO:HD3	2.22	0.40
2:B:193:ALA:HB2	2:B:208:SER:HB3	2.03	0.40
1:C:168:ALA:HA	1:C:178:LEU:HB3	2.04	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	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
1	C	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
1	E	218/226 (96%)	210 (96%)	8 (4%)	0	100	100
1	G	215/226 (95%)	207 (96%)	8 (4%)	0	100	100
2	B	210/213 (99%)	204 (97%)	6 (3%)	0	100	100
2	D	210/213 (99%)	203 (97%)	7 (3%)	0	100	100
2	F	210/213 (99%)	202 (96%)	8 (4%)	0	100	100
2	H	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
3	I	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
3	J	17/20 (85%)	16 (94%)	1 (6%)	0	100	100
All	All	1740/1796 (97%)	1676 (96%)	64 (4%)	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	181/190 (95%)	178 (98%)	3 (2%)	53	75
1	C	176/190 (93%)	169 (96%)	7 (4%)	28	61
1	E	179/190 (94%)	175 (98%)	4 (2%)	45	71
1	G	178/190 (94%)	175 (98%)	3 (2%)	53	75
2	B	181/188 (96%)	180 (99%)	1 (1%)	78	84
2	D	184/188 (98%)	181 (98%)	3 (2%)	55	75
2	F	183/188 (97%)	182 (100%)	1 (0%)	81	85
2	H	184/188 (98%)	179 (97%)	5 (3%)	39	68
3	I	14/15 (93%)	14 (100%)	0	100	100
3	J	14/15 (93%)	14 (100%)	0	100	100
All	All	1474/1542 (96%)	1447 (98%)	27 (2%)	51	74

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	169	VAL
1	A	183	THR
2	B	109	THR
1	C	1	GLN
1	C	2	VAL
1	C	22	CYS
1	C	89	VAL
1	C	183	THR
1	C	193	THR
1	C	209	LYS
2	D	158	ASN
2	D	163	VAL
2	D	183	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1	GLN
1	E	12	VAL
1	E	22	CYS
1	E	215	SER
2	F	109	THR
1	G	17	SER
1	G	18	LEU
1	G	22	CYS
2	H	1	ASP
2	H	5	THR
2	H	7	SER
2	H	163	VAL
2	H	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	82(A)	ASN
1	A	192	GLN
2	B	53	ASN
2	B	92	ASN
1	C	199	ASN
2	D	92	ASN
2	D	124	GLN
1	E	192	GLN
2	H	147	GLN
2	H	155	GLN
2	H	158	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 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	$\# Z > 2$
5	PEG	E	305	-	6,6,6	0.50	0	5,5,5	0.28	0
4	EDO	B	302	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	E	304	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	C	301	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	E	301	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	A	301	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	C	302	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	D	307	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	I	103	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	J	101	-	3,3,3	0.43	0	2,2,2	0.35	0
5	PEG	B	312	-	6,6,6	0.50	0	5,5,5	0.28	0
4	EDO	B	304	-	3,3,3	0.42	0	2,2,2	0.38	0
5	PEG	B	313	-	6,6,6	0.50	0	5,5,5	0.27	0
4	EDO	B	301	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	D	304	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	B	306	-	3,3,3	0.43	0	2,2,2	0.38	0
5	PEG	F	308	-	6,6,6	0.50	0	5,5,5	0.30	0
4	EDO	B	309	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	C	303	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	H	301	-	3,3,3	0.42	0	2,2,2	0.37	0
5	PEG	F	309	-	6,6,6	0.51	0	5,5,5	0.27	0
4	EDO	B	310	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	B	311	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	D	303	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	D	306	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	308	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	I	102	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	B	305	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	B	307	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	E	302	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	I	101	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	D	305	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	G	301	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	D	308	-	3,3,3	0.43	0	2,2,2	0.09	0
4	EDO	H	304	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	H	302	-	3,3,3	0.43	0	2,2,2	0.45	0
4	EDO	H	303	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	F	304	-	3,3,3	0.43	0	2,2,2	0.30	0
4	EDO	D	301	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	F	303	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	F	307	-	3,3,3	0.37	0	2,2,2	0.44	0
4	EDO	E	303	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	F	301	-	3,3,3	0.39	0	2,2,2	0.45	0
4	EDO	F	306	-	3,3,3	0.43	0	2,2,2	0.39	0
5	PEG	C	304	-	6,6,6	0.49	0	5,5,5	0.33	0
5	PEG	A	305	-	6,6,6	0.50	0	5,5,5	0.26	0
4	EDO	B	303	-	3,3,3	0.42	0	2,2,2	0.37	0
5	PEG	D	309	-	6,6,6	0.50	0	5,5,5	0.44	0
4	EDO	F	305	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	A	304	-	3,3,3	0.42	0	2,2,2	0.36	0
4	EDO	F	302	-	3,3,3	0.42	0	2,2,2	0.36	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
5	PEG	E	305	-	-	0/4/4/4	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	E	304	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	E	301	-	-	0/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
4	EDO	D	307	-	-	0/1/1/1	-
4	EDO	I	103	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	J	101	-	-	0/1/1/1	-
5	PEG	B	312	-	-	0/4/4/4	-
4	EDO	B	304	-	-	0/1/1/1	-
5	PEG	B	313	-	-	3/4/4/4	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
4	EDO	B	306	-	-	0/1/1/1	-
5	PEG	F	308	-	-	3/4/4/4	-
4	EDO	B	309	-	-	0/1/1/1	-
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	H	301	-	-	0/1/1/1	-
5	PEG	F	309	-	-	4/4/4/4	-
4	EDO	B	310	-	-	0/1/1/1	-
4	EDO	B	311	-	-	0/1/1/1	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	D	306	-	-	0/1/1/1	-
4	EDO	B	308	-	-	0/1/1/1	-
4	EDO	I	102	-	-	0/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	B	307	-	-	0/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-
4	EDO	I	101	-	-	0/1/1/1	-
4	EDO	D	305	-	-	0/1/1/1	-
4	EDO	G	301	-	-	0/1/1/1	-
4	EDO	D	308	-	-	0/1/1/1	-
4	EDO	H	304	-	-	0/1/1/1	-
4	EDO	H	302	-	-	0/1/1/1	-
4	EDO	H	303	-	-	0/1/1/1	-
4	EDO	F	304	-	-	0/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	F	303	-	-	0/1/1/1	-
4	EDO	D	302	-	-	0/1/1/1	-
4	EDO	F	307	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	F	301	-	-	0/1/1/1	-
4	EDO	F	306	-	-	0/1/1/1	-
5	PEG	C	304	-	-	3/4/4/4	-
5	PEG	A	305	-	-	4/4/4/4	-
4	EDO	B	303	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	309	-	-	2/4/4/4	-
4	EDO	F	305	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	F	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	304	PEG	C1-C2-O2-C3
5	B	313	PEG	O2-C3-C4-O4
5	C	304	PEG	O1-C1-C2-O2
5	F	309	PEG	O1-C1-C2-O2
5	A	305	PEG	O2-C3-C4-O4
5	F	308	PEG	O2-C3-C4-O4
5	F	309	PEG	O2-C3-C4-O4
5	A	305	PEG	C4-C3-O2-C2
5	B	313	PEG	O1-C1-C2-O2
5	F	308	PEG	O1-C1-C2-O2
5	C	304	PEG	O2-C3-C4-O4
5	F	309	PEG	C4-C3-O2-C2
5	F	308	PEG	C1-C2-O2-C3
4	B	301	EDO	O1-C1-C2-O2
5	A	305	PEG	C1-C2-O2-C3
5	A	305	PEG	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
5	F	309	PEG	C1-C2-O2-C3
5	B	313	PEG	C4-C3-O2-C2
5	D	309	PEG	O1-C1-C2-O2
5	D	309	PEG	O2-C3-C4-O4

There are no ring outliers.

17 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	EDO	1	0
4	J	101	EDO	1	0
5	B	313	PEG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	EDO	1	0
4	H	301	EDO	1	0
5	F	309	PEG	1	0
4	D	303	EDO	1	0
4	B	308	EDO	2	0
4	B	307	EDO	1	0
4	D	305	EDO	1	0
4	H	304	EDO	1	0
4	E	303	EDO	1	0
5	C	304	PEG	3	0
5	A	305	PEG	1	0
4	B	303	EDO	1	0
5	D	309	PEG	2	0
4	A	304	EDO	2	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	220/226 (97%)	-0.14	3 (1%) 73 54	41, 72, 124, 153	0
1	C	220/226 (97%)	-0.11	1 (0%) 87 76	44, 75, 118, 168	0
1	E	222/226 (98%)	0.39	3 (1%) 73 54	70, 105, 129, 203	0
1	G	219/226 (96%)	0.25	2 (0%) 81 64	63, 96, 135, 156	0
2	B	212/213 (99%)	-0.07	0 100 100	39, 64, 135, 147	0
2	D	212/213 (99%)	-0.25	0 100 100	37, 63, 88, 107	0
2	F	212/213 (99%)	0.06	4 (1%) 66 46	39, 68, 129, 140	0
2	H	213/213 (100%)	0.01	0 100 100	54, 80, 103, 119	0
3	I	19/20 (95%)	0.40	2 (10%) 11 8	48, 57, 119, 135	0
3	J	19/20 (95%)	0.42	1 (5%) 32 20	71, 88, 153, 160	0
All	All	1768/1796 (98%)	0.03	16 (0%) 81 64	37, 79, 127, 203	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	SER	4.6
1	C	215	SER	3.9
1	A	132	SER	3.3
3	I	20	PRO	3.1
1	G	214	LYS	3.0
3	J	20	PRO	2.8
3	I	2	ALA	2.7
1	E	129	LYS	2.7
1	G	134	GLY	2.5
1	E	127	SER	2.4
2	F	188	LYS	2.3
2	F	213	GLU	2.3
1	A	128	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	203	SER	2.1
1	A	213	PRO	2.1
2	F	129	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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
4	EDO	F	306	4/4	0.36	0.19	91,98,98,99	0
4	EDO	H	304	4/4	0.58	0.33	94,119,119,129	0
4	EDO	D	306	4/4	0.61	0.20	72,72,79,90	0
4	EDO	D	307	4/4	0.65	0.20	98,106,107,109	0
4	EDO	E	304	4/4	0.70	0.18	85,90,94,95	0
4	EDO	A	302	4/4	0.71	0.22	85,88,91,91	0
5	PEG	D	309	7/7	0.72	0.30	97,109,116,123	0
4	EDO	I	102	4/4	0.73	0.38	69,81,88,95	0
4	EDO	J	101	4/4	0.74	0.43	86,88,92,93	0
4	EDO	B	308	4/4	0.74	0.15	103,103,103,105	0
4	EDO	B	306	4/4	0.75	0.20	67,85,102,107	0
4	EDO	E	302	4/4	0.75	0.28	95,95,104,106	0
4	EDO	F	304	4/4	0.77	0.33	90,95,96,100	0
5	PEG	A	305	7/7	0.78	0.33	60,91,107,108	0
4	EDO	D	301	4/4	0.78	0.24	80,84,92,94	0
4	EDO	B	305	4/4	0.79	0.35	84,86,96,102	0
4	EDO	F	305	4/4	0.79	0.15	72,76,80,81	0
4	EDO	E	301	4/4	0.80	0.18	85,89,91,94	0
4	EDO	D	304	4/4	0.80	0.24	70,84,96,99	0
5	PEG	B	312	7/7	0.80	0.21	73,99,106,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	I	103	4/4	0.80	0.17	87,94,96,101	0
4	EDO	C	303	4/4	0.81	0.31	100,102,102,103	0
4	EDO	H	301	4/4	0.82	0.15	92,93,98,99	0
4	EDO	F	303	4/4	0.83	0.19	65,76,76,84	0
4	EDO	D	302	4/4	0.83	0.17	83,84,87,90	0
5	PEG	B	313	7/7	0.83	0.26	94,107,109,140	0
4	EDO	F	302	4/4	0.83	0.16	82,83,87,91	0
4	EDO	H	302	4/4	0.84	0.17	73,76,80,85	0
4	EDO	B	302	4/4	0.84	0.24	81,87,92,96	0
4	EDO	I	101	4/4	0.84	0.24	76,78,83,83	0
4	EDO	F	307	4/4	0.84	0.26	91,97,98,104	0
4	EDO	B	307	4/4	0.84	0.19	79,85,85,86	0
5	PEG	E	305	7/7	0.84	0.14	75,89,97,97	0
4	EDO	B	310	4/4	0.85	0.31	98,100,105,111	0
4	EDO	A	303	4/4	0.85	0.16	88,99,107,116	0
4	EDO	G	301	4/4	0.85	0.21	88,92,96,99	0
5	PEG	F	309	7/7	0.85	0.26	100,103,123,123	0
4	EDO	B	309	4/4	0.86	0.17	67,70,78,92	0
4	EDO	C	301	4/4	0.86	0.33	83,90,91,93	0
5	PEG	C	304	7/7	0.86	0.30	71,91,99,100	0
5	PEG	F	308	7/7	0.87	0.16	66,81,83,84	0
4	EDO	F	301	4/4	0.87	0.27	80,96,99,102	0
4	EDO	A	304	4/4	0.88	0.21	86,86,91,94	0
4	EDO	D	305	4/4	0.88	0.20	53,74,86,91	0
4	EDO	B	303	4/4	0.88	0.18	72,86,87,95	0
4	EDO	B	311	4/4	0.89	0.30	104,105,107,108	0
4	EDO	E	303	4/4	0.90	0.20	91,94,97,98	0
4	EDO	C	302	4/4	0.91	0.27	66,87,89,98	0
4	EDO	D	303	4/4	0.91	0.25	73,86,89,97	0
4	EDO	H	303	4/4	0.91	0.20	89,96,106,108	0
4	EDO	D	308	4/4	0.91	0.22	90,97,98,104	0
4	EDO	A	301	4/4	0.92	0.17	67,74,89,89	0
4	EDO	B	301	4/4	0.93	0.15	65,66,68,76	0
4	EDO	B	304	4/4	0.93	0.15	73,78,79,85	0

6.5 Other polymers ⓘ

There are no such residues in this entry.