



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:09 AM UTC

PDB ID : 7Q98 / pdb_00007q98
Title : MHC Class I A02 Allele presenting NLSALGIFST
Authors : Rizkallah, P.J.; Sewell, A.K.
Deposited on : 2021-11-12
Resolution : 2.50 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

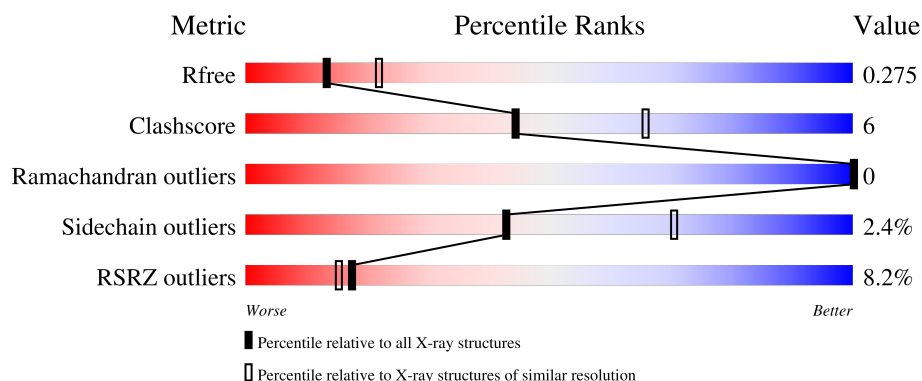
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	276	14% 84% 13% .
1	D	276	8% 86% 14%
1	G	276	13% 87% 13%
1	J	276	5% 87% 13%
1	M	276	12% 86% 14%

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Mol	Chain	Length	Quality of chain
2	B	100	4% 86% 14%
2	E	100	3% 88% 12%
2	H	100	84% 16%
2	K	100	81% 18%
2	N	100	79% 20%
3	C	10	50% 70% 20% 10%
3	F	10	90% 10%
3	I	10	70% 30%
3	L	10	10% 90% 10%
3	O	10	20% 70% 30%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16557 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	D	276	Total	C	N	O	S	0	1	0
			2262	1413	411	428	10			
1	G	276	Total	C	N	O	S	0	1	0
			2262	1413	411	428	10			
1	J	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			
1	M	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			
2	E	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	K	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	N	100	Total	C	N	O	S	0	1	0
			848	539	145	160	4			

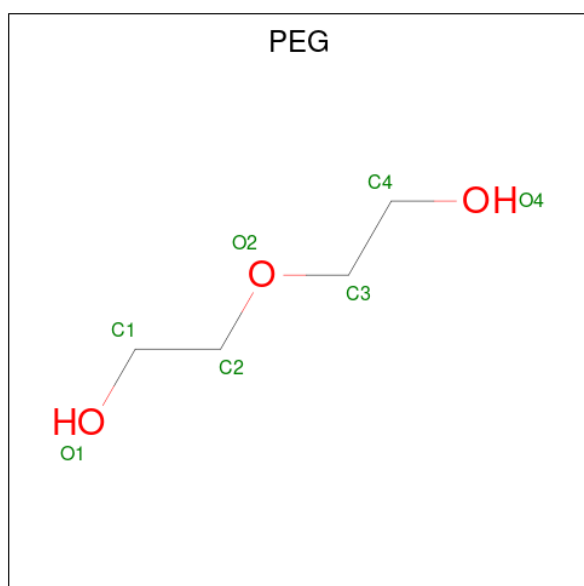
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769
H	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
N	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			72	46	11	15			
3	F	10	Total	C	N	O	0	0	0
			72	46	11	15			
3	I	10	Total	C	N	O	0	0	0
			72	46	11	15			
3	L	10	Total	C	N	O	0	0	0
			72	46	11	15			
3	O	10	Total	C	N	O	0	0	0
			72	46	11	15			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



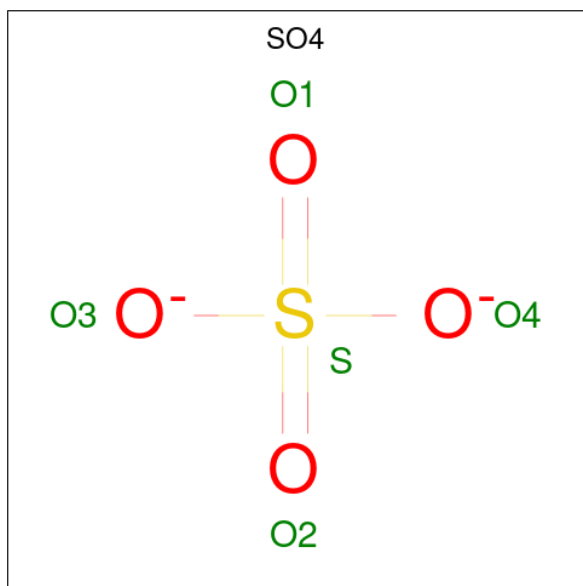
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		
4	J	1	Total	C	O	0	0
			7	4	3		
4	K	1	Total	C	O	0	0
			7	4	3		
4	N	1	Total	C	O	0	0
			7	4	3		
4	N	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



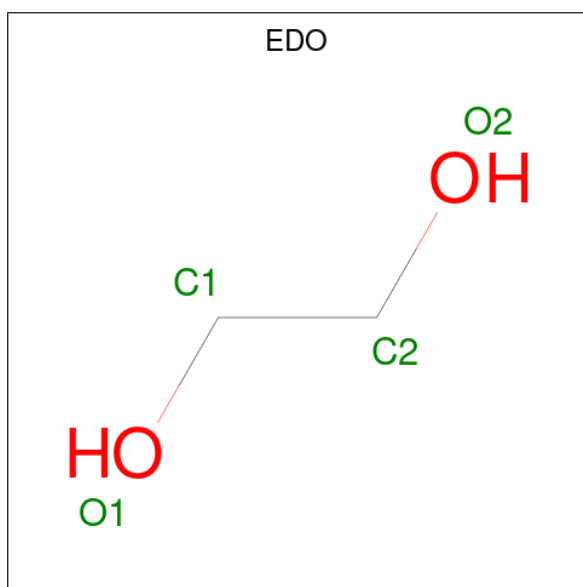
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	J	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	M	1	Total	C	O	0	0
			4	2	2		
6	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	43	Total	O	0	0
			43	43		
7	B	29	Total	O	0	0
			29	29		
7	C	3	Total	O	0	0
			3	3		
7	D	83	Total	O	0	0
			83	83		
7	E	33	Total	O	0	0
			33	33		
7	F	3	Total	O	0	0
			3	3		
7	G	50	Total	O	0	0
			50	50		
7	H	32	Total	O	0	0
			32	32		

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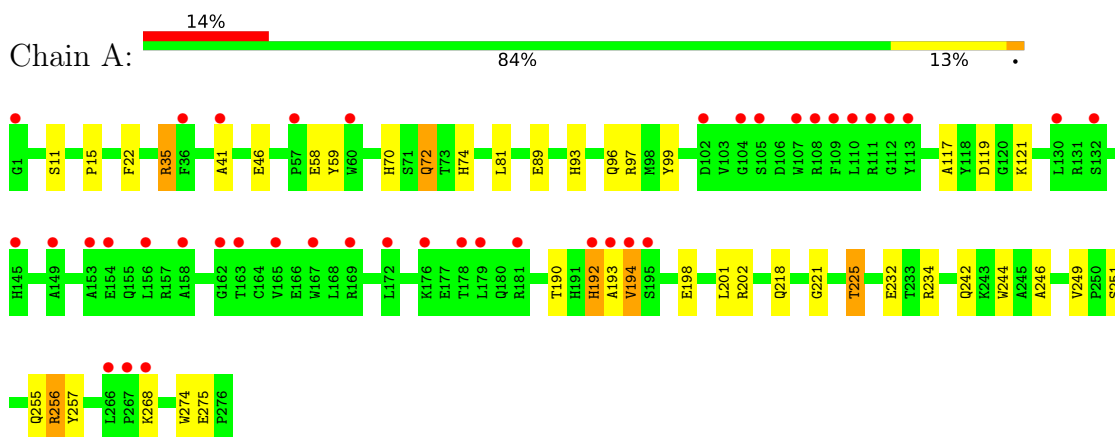
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	2	Total 2	O 2	0	0
7	J	22	Total 22	O 22	0	0
7	K	38	Total 38	O 38	0	0
7	L	2	Total 2	O 2	0	0
7	M	67	Total 67	O 67	0	0
7	N	58	Total 58	O 58	0	0
7	O	2	Total 2	O 2	0	0

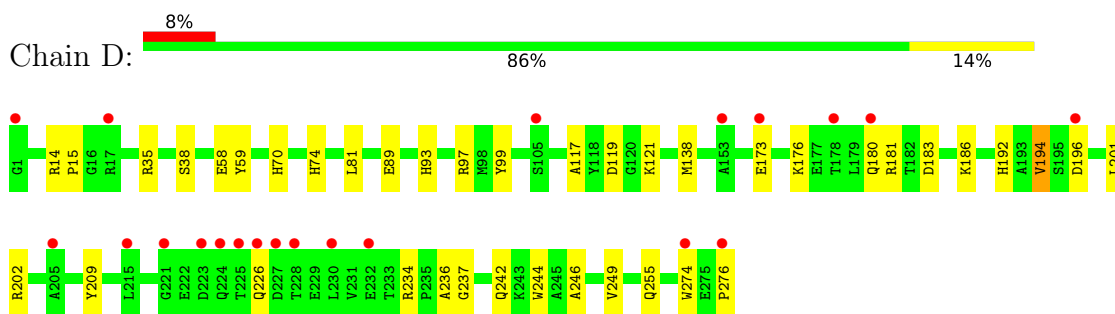
3 Residue-property plots [i](#)

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.

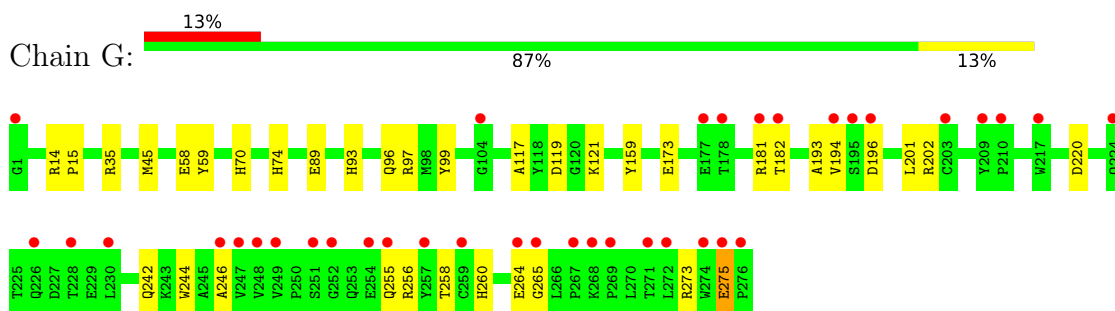
- Molecule 1: MHC class I antigen



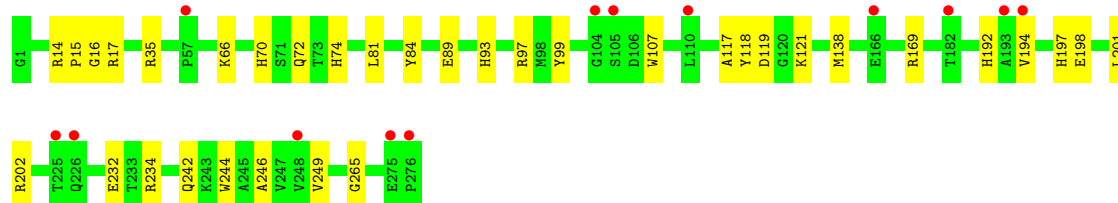
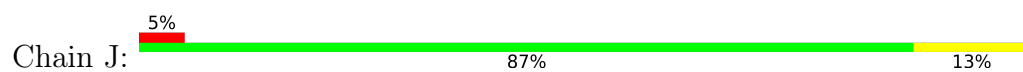
- Molecule 1: MHC class I antigen



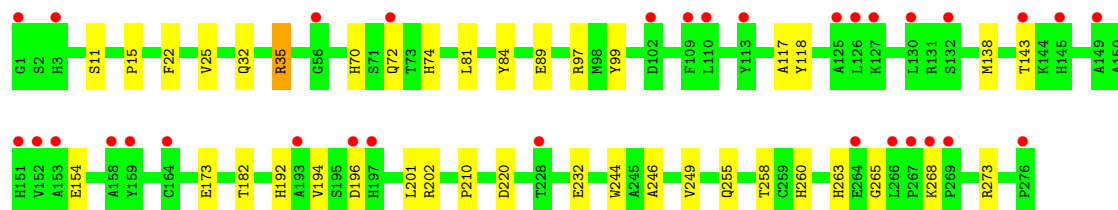
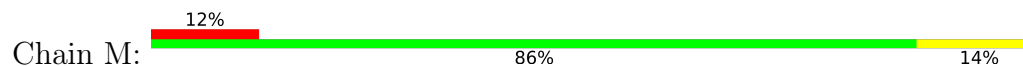
- Molecule 1: MHC class I antigen



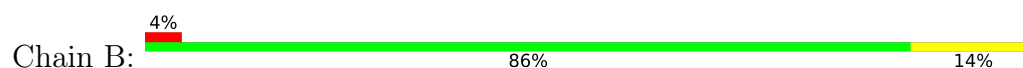
- Molecule 1: MHC class I antigen



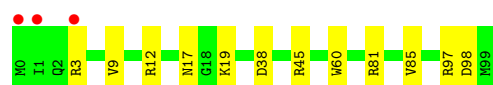
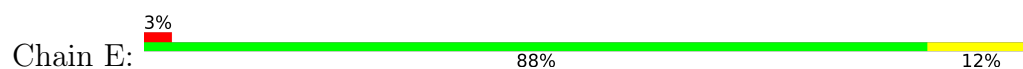
- Molecule 1: MHC class I antigen



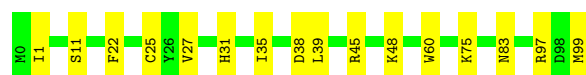
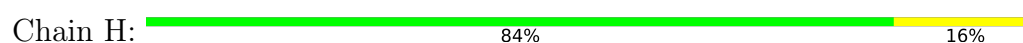
- Molecule 2: Beta-2-microglobulin



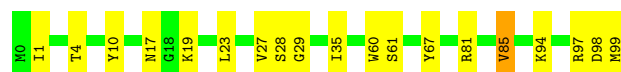
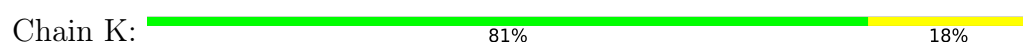
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

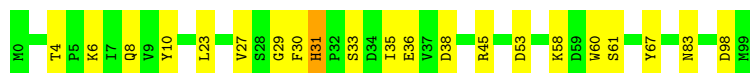


- Molecule 2: Beta-2-microglobulin



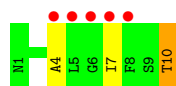
- Molecule 2: Beta-2-microglobulin

Chain N:  79% 20% .



- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain C:  50% 70% 20% 10%



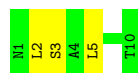
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain F:  90% 10%



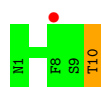
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain I:  70% 30%



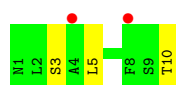
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain L:  10% 90% 10%



- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain O:  20% 70% 30%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.25Å 169.69Å 248.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.00 – 2.50 85.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (85.00-2.50) 99.0 (85.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.274 0.238 , 0.275	Depositor DCC
R_{free} test set	4345 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16557	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.75 % 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 5.7511e-06. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, 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	1.07	1/2320 (0.0%)	1.34	1/3149 (0.0%)
1	D	1.12	1/2328 (0.0%)	1.38	3/3159 (0.1%)
1	G	1.05	0/2328	1.32	1/3159 (0.0%)
1	J	1.04	0/2320	1.32	0/3149
1	M	1.10	0/2320	1.34	0/3149
2	B	1.02	0/871	1.20	0/1176
2	E	1.05	0/871	1.23	0/1176
2	H	1.01	0/860	1.20	0/1162
2	K	1.06	0/860	1.19	1/1162 (0.1%)
2	N	1.14	2/871 (0.2%)	1.22	1/1176 (0.1%)
3	C	1.17	0/72	1.52	0/95
3	F	1.26	0/72	1.54	0/95
3	I	0.90	0/72	1.51	0/95
3	L	1.21	0/72	1.41	0/95
3	O	1.16	0/72	1.55	0/95
All	All	1.07	4/16309 (0.0%)	1.31	7/22092 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	31	HIS	CE1-NE2	6.40	1.39	1.32
1	A	192	HIS	CE1-NE2	5.91	1.38	1.32
2	N	33	SER	C-O	-5.51	1.17	1.24
1	D	121	LYS	C-O	-5.11	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	THR	CA-CB-OG1	-7.97	97.64	109.60
1	D	196	ASP	CA-CB-CG	6.61	119.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	226	GLN	CA-C-O	-5.25	114.85	120.42
2	N	4	THR	CB-CA-C	5.05	116.68	109.26
1	D	194	VAL	N-CA-C	-5.01	107.95	112.96
2	K	4	THR	CB-CA-C	5.00	116.61	109.26

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	2254	0	2103	28	0
1	D	2262	0	2111	25	0
1	G	2262	0	2111	25	0
1	J	2254	0	2103	28	0
1	M	2254	0	2103	32	0
2	B	848	0	815	17	0
2	E	848	0	815	16	0
2	H	837	0	803	15	0
2	K	837	0	803	17	0
2	N	848	0	815	17	0
3	C	72	0	75	4	0
3	F	72	0	75	2	0
3	I	72	0	75	4	0
3	L	72	0	75	1	0
3	O	72	0	75	4	0
4	A	14	0	20	1	0
4	B	7	0	10	2	0
4	D	21	0	30	0	0
4	E	7	0	10	1	0
4	G	21	0	30	1	0
4	H	7	0	10	2	0
4	J	7	0	10	1	0
4	K	7	0	10	2	0
4	N	14	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	0	1	0
5	D	35	0	0	2	0
5	E	10	0	0	1	0
5	G	20	0	0	0	0
5	H	5	0	0	1	0
5	J	10	0	0	1	0
5	K	10	0	0	1	0
5	N	5	0	0	0	0
6	B	4	0	6	0	0
6	D	4	0	6	1	0
6	M	4	0	6	0	0
6	N	4	0	6	0	0
7	A	43	0	0	4	0
7	B	29	0	0	3	0
7	C	3	0	0	1	0
7	D	83	0	0	1	0
7	E	33	0	0	1	0
7	F	3	0	0	0	0
7	G	50	0	0	0	0
7	H	32	0	0	3	0
7	I	2	0	0	0	0
7	J	22	0	0	0	0
7	K	38	0	0	2	0
7	L	2	0	0	0	0
7	M	67	0	0	4	0
7	N	58	0	0	2	0
7	O	2	0	0	0	0
All	All	16557	0	15131	188	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 6.

All (188) 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)
2:E:38:ASP:OD2	2:E:45:ARG:HD2	1.62	1.00
2:N:31:HIS:HD2	7:N:206:HOH:O	1.50	0.92
1:A:35:ARG:NH2	1:A:46:GLU:OE2	2.04	0.90
1:M:192:HIS:HE1	2:N:98:ASP:OD2	1.57	0.87
1:D:180:GLN:NE2	1:D:183:ASP:OD2	2.10	0.84
2:N:10:TYR:HB2	4:N:101:PEG:H22	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ASP:OD2	1:J:138:MET:SD	2.41	0.79
1:D:138[B]:MET:HE3	2:K:81:ARG:HD2	1.65	0.77
1:M:154:GLU:HA	7:M:412:HOH:O	1.85	0.76
2:B:7:ILE:HD12	2:B:82:VAL:HG21	1.67	0.76
3:C:7:ILE:O	3:C:7:ILE:HG22	1.84	0.76
2:H:99:MET:HE2	5:H:102:SO4:O3	1.86	0.75
7:A:441:HOH:O	2:B:98:ASP:HB2	1.86	0.75
2:B:81[A]:ARG:HH21	1:J:138:MET:HE2	1.50	0.75
4:B:101:PEG:H41	7:B:228:HOH:O	1.84	0.75
1:A:192:HIS:NE2	2:B:98:ASP:OD2	2.21	0.74
1:J:192:HIS:NE2	2:K:98:ASP:OD2	2.15	0.71
1:M:210:PRO:O	1:M:263:HIS:HE1	1.75	0.69
2:N:8:GLN:HE21	4:N:102:PEG:H42	1.57	0.69
1:D:81:LEU:HD21	3:F:10:THR:HG21	1.75	0.67
2:E:9:VAL:O	5:E:102:SO4:O3	2.14	0.66
2:E:38:ASP:OD2	2:E:45:ARG:CD	2.42	0.66
1:M:81:LEU:HD21	3:O:10:THR:HG21	1.78	0.66
1:D:138[B]:MET:HE3	2:K:81:ARG:CD	2.26	0.65
1:D:192:HIS:HE1	2:E:98:ASP:OD2	1.80	0.64
3:C:4:ALA:HB1	7:C:103:HOH:O	1.97	0.64
2:K:10:TYR:HB2	4:K:101:PEG:H22	1.80	0.63
1:D:234:ARG:HE	1:D:242:GLN:HE21	1.46	0.61
2:E:81:ARG:NE	1:M:138:MET:HE2	2.16	0.61
2:E:45:ARG:NH1	1:M:84:TYR:O	2.32	0.61
2:E:81:ARG:NH1	1:M:138:MET:HG2	2.16	0.61
1:A:232:GLU:H	4:B:101:PEG:H42	1.66	0.61
3:O:3:SER:OG	3:O:5:LEU:HD23	2.00	0.61
1:M:192:HIS:CE1	2:N:98:ASP:OD2	2.48	0.60
1:D:93:HIS:HD2	1:D:119:ASP:OD2	1.85	0.60
2:N:27:VAL:HG11	2:N:35:ILE:HD13	1.83	0.59
1:G:220:ASP:OD2	1:G:256:ARG:NH2	2.37	0.58
2:E:3[A]:ARG:NH2	1:J:16:GLY:O	2.37	0.58
2:B:31:HIS:HD2	7:B:211:HOH:O	1.85	0.57
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.57
1:A:251:SER:OG	5:A:304:SO4:O2	2.22	0.57
1:G:202:ARG:HD3	1:G:244:TRP:CD2	2.39	0.57
1:G:93:HIS:HD2	1:G:119:ASP:OD2	1.87	0.57
1:J:197:HIS:NE2	1:J:198:GLU:OE2	2.38	0.57
1:J:93:HIS:HD2	1:J:119:ASP:OD2	1.88	0.57
2:N:31:HIS:CD2	7:N:206:HOH:O	2.38	0.56
1:J:121:LYS:HG3	2:K:1:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:234:ARG:HE	1:J:242:GLN:HE21	1.53	0.56
2:K:27:VAL:HG11	2:K:35:ILE:HD13	1.87	0.56
2:E:38:ASP:CG	1:M:138:MET:SD	2.89	0.56
1:G:96:GLN:OE1	2:H:31:HIS:HE1	1.89	0.56
1:M:154:GLU:CA	7:M:412:HOH:O	2.49	0.55
2:B:81[A]:ARG:HD3	1:J:138:MET:HE2	1.87	0.55
1:G:255:GLN:H	1:G:255:GLN:CD	2.13	0.55
1:M:74:HIS:CE1	1:M:97:ARG:HE	2.25	0.55
1:M:143:THR:OG1	3:O:10:THR:HG23	2.07	0.55
1:A:96:GLN:OE1	2:B:31:HIS:HE1	1.90	0.55
1:A:255:GLN:OE1	1:A:274:TRP:O	2.25	0.55
1:M:11:SER:OG	1:M:22:PHE:HD1	1.89	0.55
1:J:107:TRP:O	1:J:169:ARG:CZ	2.55	0.55
2:H:31:HIS:HD2	7:H:215:HOH:O	1.90	0.54
1:A:74:HIS:CE1	1:A:97:ARG:HE	2.26	0.54
2:H:27:VAL:HG11	2:H:35:ILE:HD13	1.90	0.54
2:H:97:ARG:NH2	7:H:203:HOH:O	2.41	0.54
2:H:38:ASP:OD2	2:H:45:ARG:HD2	2.08	0.54
1:D:74:HIS:CE1	1:D:97:ARG:HE	2.26	0.53
2:E:3[A]:ARG:NH2	1:J:17:ARG:HA	2.23	0.53
3:I:5:LEU:HD23	3:I:5:LEU:N	2.24	0.53
1:G:74:HIS:CE1	1:G:97:ARG:HE	2.27	0.53
1:J:74:HIS:CE1	1:J:97:ARG:HE	2.27	0.53
2:N:27:VAL:HG11	2:N:35:ILE:CD1	2.39	0.53
1:D:81:LEU:CD2	3:F:10:THR:HG21	2.39	0.52
1:A:11:SER:OG	1:A:22:PHE:HD1	1.91	0.52
1:A:192:HIS:CE1	2:B:98:ASP:OD2	2.62	0.52
1:D:70:HIS:HE1	1:D:99:TYR:OH	1.92	0.52
2:B:27:VAL:HG11	2:B:35:ILE:HD13	1.92	0.52
2:E:17:ASN:OD1	2:E:97:ARG:NH2	2.38	0.52
1:D:38:SER:OG	5:D:310:SO4:O2	2.19	0.52
2:N:6:LYS:HB3	4:N:102:PEG:H31	1.91	0.51
1:A:70:HIS:HE1	1:A:99:TYR:OH	1.94	0.51
1:G:181:ARG:NH2	1:J:265:GLY:O	2.43	0.51
2:K:17:ASN:OD1	2:K:97:ARG:NH2	2.40	0.51
1:G:58:GLU:HG2	1:G:59:TYR:N	2.25	0.51
1:A:41:ALA:HB3	4:J:301:PEG:H11	1.92	0.50
1:A:58:GLU:HG2	1:A:59:TYR:N	2.27	0.50
1:D:58:GLU:HG2	1:D:59:TYR:N	2.27	0.50
1:G:242:GLN:NE2	4:H:101:PEG:H31	2.26	0.50
1:D:181:ARG:HA	6:D:311:EDO:H12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:ILE:O	3:C:7:ILE:CG2	2.54	0.49
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.47	0.49
1:G:70:HIS:HE1	1:G:99:TYR:OH	1.94	0.49
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.59	0.49
2:N:38:ASP:OD2	2:N:45:ARG:HD2	2.13	0.49
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.47	0.49
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.47	0.49
1:A:72:GLN:HA	1:A:72:GLN:OE1	2.11	0.49
1:A:194:VAL:HG22	1:A:198:GLU:HB2	1.95	0.49
1:M:11:SER:HG	1:M:22:PHE:HD1	1.60	0.49
2:B:38:ASP:OD2	1:J:138:MET:HB2	2.13	0.49
2:E:97:ARG:NH1	4:E:101:PEG:O4	2.45	0.49
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.48	0.49
1:J:107:TRP:O	1:J:169:ARG:NH1	2.46	0.49
2:H:48:LYS:O	2:H:48:LYS:HG3	2.13	0.48
1:G:220:ASP:O	1:M:273:ARG:CZ	2.61	0.48
1:M:232:GLU:OE1	2:N:6:LYS:NZ	2.28	0.48
1:M:202:ARG:HD3	1:M:244:TRP:CE3	2.49	0.48
1:A:15:PRO:HB3	1:A:89:GLU:O	2.14	0.48
1:D:255:GLN:NE2	5:D:306:SO4:O4	2.47	0.48
1:D:15:PRO:HB3	1:D:89:GLU:O	2.14	0.47
1:J:202:ARG:HD3	1:J:244:TRP:CE3	2.49	0.47
1:D:236:ALA:O	2:E:12:ARG:HG3	2.13	0.47
1:G:45:MET:CE	3:I:2:LEU:HD11	2.44	0.47
1:J:15:PRO:HB3	1:J:89:GLU:O	2.14	0.47
1:M:35:ARG:NH2	2:N:53:ASP:OD1	2.46	0.47
1:M:201:LEU:O	1:M:246:ALA:HA	2.15	0.47
1:G:201:LEU:O	1:G:246:ALA:HA	2.15	0.47
1:J:70:HIS:HE1	1:J:99:TYR:OH	1.97	0.47
2:K:99:MET:OXT	4:K:101:PEG:H11	2.14	0.47
1:A:257:TYR:O	7:A:401:HOH:O	2.20	0.47
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.50	0.46
1:M:255:GLN:HB2	7:M:425:HOH:O	2.15	0.46
1:J:232:GLU:OE2	2:K:28:SER:OG	2.33	0.46
2:K:27:VAL:HG11	2:K:35:ILE:CD1	2.44	0.46
1:G:182:THR:HG21	1:G:265:GLY:CA	2.44	0.46
1:A:194:VAL:CG2	1:A:198:GLU:HB2	2.46	0.46
1:D:186:LYS:HG3	7:D:442:HOH:O	2.15	0.46
1:D:237:GLY:HA3	7:E:217:HOH:O	2.15	0.46
1:M:182:THR:HG21	1:M:265:GLY:CA	2.45	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:PRO:HB3	1:M:89:GLU:O	2.16	0.45
1:A:11:SER:HG	1:A:22:PHE:HD1	1.63	0.45
1:M:173:GLU:HA	1:M:173:GLU:OE2	2.17	0.45
1:A:256:ARG:HD2	7:A:428:HOH:O	2.16	0.45
1:A:81:LEU:HD21	3:C:10:THR:HG21	1.99	0.45
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.82	0.44
2:E:81:ARG:CD	1:M:138:MET:HE2	2.46	0.44
1:G:273:ARG:NH1	1:M:220:ASP:CG	2.75	0.44
1:J:201:LEU:O	1:J:246:ALA:HA	2.18	0.44
2:K:85:VAL:HG22	7:K:210:HOH:O	2.17	0.44
1:M:25:VAL:CG2	1:M:32:GLN:HG3	2.47	0.44
1:M:117:ALA:HB2	2:N:60:TRP:CE2	2.52	0.44
2:B:45:ARG:NH2	1:J:84:TYR:O	2.42	0.44
7:B:224:HOH:O	1:J:138:MET:HG2	2.18	0.44
1:G:15:PRO:HB3	1:G:89:GLU:O	2.17	0.44
1:G:121:LYS:HB2	2:H:1:ILE:HD13	2.00	0.44
1:D:173:GLU:OE2	1:D:173:GLU:HA	2.18	0.43
1:D:201:LEU:O	1:D:246:ALA:HA	2.19	0.43
2:B:20:SER:HA	2:B:71:THR:HG22	2.01	0.43
2:K:97:ARG:NH1	7:K:204:HOH:O	2.50	0.43
2:N:23:LEU:O	2:N:67:TYR:HA	2.19	0.43
1:G:193:ALA:HB2	4:G:302:PEG:C2	2.49	0.43
1:M:263:HIS:CD2	1:M:265:GLY:H	2.37	0.43
1:G:275:GLU:HG2	2:K:19:LYS:CE	2.49	0.42
2:N:29:GLY:HA2	2:N:61:SER:OG	2.18	0.42
1:M:70:HIS:HE1	1:M:99:TYR:OH	2.02	0.42
2:E:3[B]:ARG:HH11	2:E:3[B]:ARG:HD3	1.72	0.42
2:N:36:GLU:HB2	2:N:83:ASN:HB3	2.02	0.42
1:A:190:THR:HG22	4:A:302:PEG:H21	2.00	0.42
2:K:23:LEU:O	2:K:67:TYR:HA	2.20	0.42
2:K:94:LYS:O	5:K:102:SO4:O3	2.38	0.42
1:M:81:LEU:HD13	1:M:118:TYR:CD1	2.55	0.42
1:D:180:GLN:HG3	1:D:209:TYR:CG	2.54	0.42
1:G:45:MET:HE2	3:I:2:LEU:HD11	2.00	0.42
2:H:31:HIS:CD2	7:H:215:HOH:O	2.70	0.42
1:J:66:LYS:NZ	5:J:303:SO4:O1	2.37	0.42
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.55	0.42
1:M:154:GLU:N	7:M:412:HOH:O	2.53	0.41
1:M:258:THR:OG1	1:M:260:HIS:HE1	2.02	0.41
1:A:201:LEU:O	1:A:246:ALA:HA	2.20	0.41
2:B:81[A]:ARG:HD3	1:J:138:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:ASN:HD22	2:H:83:ASN:HA	1.63	0.41
1:G:258:THR:OG1	1:G:260:HIS:HE1	2.03	0.41
1:A:193:ALA:HB1	7:A:433:HOH:O	2.20	0.41
1:D:234:ARG:HE	1:D:242:GLN:NE2	2.16	0.41
1:D:274:TRP:CZ2	1:D:276:PRO:HB3	2.55	0.41
2:B:38:ASP:OD2	1:J:138:MET:CB	2.69	0.41
2:K:29:GLY:HA2	2:K:61:SER:OG	2.20	0.41
3:O:5:LEU:HD23	3:O:5:LEU:N	2.36	0.41
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.51	0.41
2:N:27:VAL:HG12	2:N:30:PHE:CE1	2.56	0.41
2:H:99:MET:OXT	4:H:101:PEG:H11	2.21	0.40
1:G:173:GLU:OE2	1:G:173:GLU:HA	2.21	0.40
1:G:182:THR:HG21	1:G:265:GLY:HA2	2.03	0.40
1:G:159:TYR:CD1	3:I:3:SER:HA	2.57	0.40
2:H:27:VAL:HG11	2:H:35:ILE:CD1	2.50	0.40
2:H:11:SER:HA	2:H:22:PHE:O	2.21	0.40
2:H:25:CYS:HB2	2:H:39:LEU:HD21	2.03	0.40
1:J:81:LEU:HG	3:L:10:THR:HG21	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	274/276 (99%)	270 (98%)	4 (2%)	0	100	100
1	D	275/276 (100%)	270 (98%)	5 (2%)	0	100	100
1	G	275/276 (100%)	271 (98%)	4 (2%)	0	100	100
1	J	274/276 (99%)	270 (98%)	4 (2%)	0	100	100
1	M	274/276 (99%)	270 (98%)	4 (2%)	0	100	100
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
2	H	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	K	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	N	99/100 (99%)	97 (98%)	2 (2%)	0	100	100
3	C	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	F	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	I	8/10 (80%)	8 (100%)	0	0	100	100
3	L	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	O	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	1905/1930 (99%)	1873 (98%)	32 (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	232/232 (100%)	223 (96%)	9 (4%)	28	55
1	D	233/232 (100%)	228 (98%)	5 (2%)	47	74
1	G	233/232 (100%)	228 (98%)	5 (2%)	47	74
1	J	232/232 (100%)	227 (98%)	5 (2%)	45	73
1	M	232/232 (100%)	226 (97%)	6 (3%)	40	68
2	B	96/95 (101%)	94 (98%)	2 (2%)	47	74
2	E	96/95 (101%)	94 (98%)	2 (2%)	47	74
2	H	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	K	95/95 (100%)	94 (99%)	1 (1%)	65	84
2	N	96/95 (101%)	95 (99%)	1 (1%)	68	86
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	9
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	8/8 (100%)	8 (100%)	0	100	100
3	L	8/8 (100%)	7 (88%)	1 (12%)	4	9
3	O	8/8 (100%)	8 (100%)	0	100	100
All	All	1680/1675 (100%)	1640 (98%)	40 (2%)	43	70

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	72	GLN
1	A	121	LYS
1	A	194	VAL
1	A	225	THR
1	A	249	VAL
1	A	256	ARG
1	A	268	LYS
1	A	275	GLU
2	B	9	VAL
2	B	97	ARG
3	C	10	THR
1	D	14	ARG
1	D	35	ARG
1	D	176	LYS
1	D	194	VAL
1	D	249	VAL
2	E	19	LYS
2	E	85	VAL
3	F	10	THR
1	G	14	ARG
1	G	35	ARG
1	G	194	VAL
1	G	264	GLU
1	G	275	GLU
2	H	75	LYS
1	J	14	ARG
1	J	35	ARG
1	J	72	GLN
1	J	194	VAL
1	J	249	VAL
2	K	85	VAL
3	L	10	THR

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Mol	Chain	Res	Type
1	M	35	ARG
1	M	72	GLN
1	M	194	VAL
1	M	196	ASP
1	M	249	VAL
1	M	268	LYS
2	N	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	70	HIS
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	174	ASN
1	A	180	GLN
1	A	218	GLN
1	A	242	GLN
1	A	255	GLN
1	A	260	HIS
2	B	31	HIS
2	B	83	ASN
3	C	1	ASN
1	D	32	GLN
1	D	43	GLN
1	D	70	HIS
1	D	86	ASN
1	D	87	GLN
1	D	93	HIS
1	D	174	ASN
1	D	180	GLN
1	D	188	HIS
1	D	192	HIS
1	D	242	GLN
2	E	83	ASN
2	E	89	GLN
1	G	43	GLN
1	G	70	HIS
1	G	74	HIS
1	G	86	ASN

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Mol	Chain	Res	Type
1	G	87	GLN
1	G	93	HIS
1	G	174	ASN
1	G	180	GLN
1	G	218	GLN
1	G	242	GLN
1	G	260	HIS
2	H	13	HIS
2	H	31	HIS
2	H	83	ASN
1	J	70	HIS
1	J	74	HIS
1	J	86	ASN
1	J	87	GLN
1	J	93	HIS
1	J	141	GLN
1	J	174	ASN
1	J	180	GLN
1	J	218	GLN
1	J	226	GLN
1	J	242	GLN
2	K	83	ASN
3	L	1	ASN
1	M	43	GLN
1	M	70	HIS
1	M	74	HIS
1	M	86	ASN
1	M	174	ASN
1	M	180	GLN
1	M	192	HIS
1	M	218	GLN
1	M	224	GLN
1	M	255	GLN
1	M	260	HIS
1	M	263	HIS
2	N	31	HIS
3	O	1	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

40 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	SO4	D	308	-	4,4,4	0.30	0	6,6,6	0.07	0
5	SO4	G	304	-	4,4,4	0.31	0	6,6,6	0.06	0
5	SO4	G	305	-	4,4,4	0.33	0	6,6,6	0.08	0
6	EDO	N	104	-	3,3,3	0.29	0	2,2,2	0.33	0
5	SO4	D	310	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	D	304	-	4,4,4	0.31	0	6,6,6	0.07	0
4	PEG	K	101	-	6,6,6	0.33	0	5,5,5	0.17	0
5	SO4	J	303	-	4,4,4	0.31	0	6,6,6	0.10	0
4	PEG	G	301	-	6,6,6	0.23	0	5,5,5	0.06	0
5	SO4	K	102	-	4,4,4	0.32	0	6,6,6	0.13	0
4	PEG	E	101	-	6,6,6	0.15	0	5,5,5	0.06	0
5	SO4	G	307	-	4,4,4	0.32	0	6,6,6	0.07	0
5	SO4	G	306	-	4,4,4	0.32	0	6,6,6	0.07	0
5	SO4	D	309	-	4,4,4	0.32	0	6,6,6	0.09	0
4	PEG	N	101	-	6,6,6	0.33	0	5,5,5	0.11	0
4	PEG	D	302	-	6,6,6	0.21	0	5,5,5	0.13	0
5	SO4	E	103	-	4,4,4	0.30	0	6,6,6	0.16	0
5	SO4	K	103	-	4,4,4	0.33	0	6,6,6	0.09	0
4	PEG	H	101	-	6,6,6	0.23	0	5,5,5	0.13	0
5	SO4	J	302	-	4,4,4	0.29	0	6,6,6	0.08	0
4	PEG	A	302	-	6,6,6	0.29	0	5,5,5	0.15	0
5	SO4	H	102	-	4,4,4	0.44	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	303	-	6,6,6	0.24	0	5,5,5	0.09	0
5	SO4	N	103	-	4,4,4	0.25	0	6,6,6	0.07	0
6	EDO	D	311	-	3,3,3	0.25	0	2,2,2	0.26	0
5	SO4	E	102	-	4,4,4	0.46	0	6,6,6	0.18	0
5	SO4	D	305	-	4,4,4	0.30	0	6,6,6	0.09	0
4	PEG	N	102	-	6,6,6	0.52	0	5,5,5	0.26	0
4	PEG	A	301	-	6,6,6	0.32	0	5,5,5	0.16	0
5	SO4	A	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	PEG	G	302	-	6,6,6	0.36	0	5,5,5	0.17	0
4	PEG	D	301	-	6,6,6	0.27	0	5,5,5	0.09	0
4	PEG	J	301	-	6,6,6	0.19	0	5,5,5	0.07	0
6	EDO	B	102	-	3,3,3	0.12	0	2,2,2	0.09	0
4	PEG	B	101	-	6,6,6	0.38	0	5,5,5	0.23	0
5	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.10	0
5	SO4	D	307	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SO4	D	306	-	4,4,4	0.34	0	6,6,6	0.08	0
4	PEG	G	303	-	6,6,6	0.20	0	5,5,5	0.11	0
6	EDO	M	301	-	3,3,3	0.17	0	2,2,2	0.22	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
6	EDO	N	104	-	-	0/1/1/1	-
4	PEG	K	101	-	-	1/4/4/4	-
4	PEG	G	301	-	-	2/4/4/4	-
4	PEG	E	101	-	-	2/4/4/4	-
4	PEG	N	101	-	-	4/4/4/4	-
4	PEG	D	302	-	-	3/4/4/4	-
4	PEG	H	101	-	-	3/4/4/4	-
4	PEG	A	302	-	-	4/4/4/4	-
4	PEG	D	303	-	-	1/4/4/4	-
6	EDO	D	311	-	-	1/1/1/1	-
4	PEG	N	102	-	-	3/4/4/4	-
4	PEG	A	301	-	-	3/4/4/4	-
4	PEG	G	302	-	-	3/4/4/4	-
4	PEG	D	301	-	-	1/4/4/4	-
4	PEG	J	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	102	-	-	1/1/1/1	-
4	PEG	B	101	-	-	1/4/4/4	-
4	PEG	G	303	-	-	3/4/4/4	-
6	EDO	M	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	302	PEG	O1-C1-C2-O2
4	G	301	PEG	O2-C3-C4-O4
4	G	303	PEG	O2-C3-C4-O4
4	A	301	PEG	O1-C1-C2-O2
4	A	301	PEG	O2-C3-C4-O4
4	H	101	PEG	O1-C1-C2-O2
4	G	302	PEG	O1-C1-C2-O2
4	N	102	PEG	O1-C1-C2-O2
4	N	102	PEG	O2-C3-C4-O4
6	D	311	EDO	O1-C1-C2-O2
6	M	301	EDO	O1-C1-C2-O2
4	A	302	PEG	O1-C1-C2-O2
4	J	301	PEG	O1-C1-C2-O2
4	N	101	PEG	O1-C1-C2-O2
4	N	101	PEG	O2-C3-C4-O4
4	K	101	PEG	O1-C1-C2-O2
4	J	301	PEG	O2-C3-C4-O4
6	B	102	EDO	O1-C1-C2-O2
4	A	302	PEG	C4-C3-O2-C2
4	D	303	PEG	C4-C3-O2-C2
4	N	101	PEG	C1-C2-O2-C3
4	A	302	PEG	O2-C3-C4-O4
4	G	301	PEG	O1-C1-C2-O2
4	G	302	PEG	C1-C2-O2-C3
4	D	302	PEG	C4-C3-O2-C2
4	G	303	PEG	C4-C3-O2-C2
4	N	102	PEG	C1-C2-O2-C3
4	B	101	PEG	C1-C2-O2-C3
4	D	301	PEG	C4-C3-O2-C2
4	E	101	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	D	302	PEG	O2-C3-C4-O4
4	G	302	PEG	O2-C3-C4-O4
4	N	101	PEG	C4-C3-O2-C2
4	H	101	PEG	C4-C3-O2-C2
4	A	301	PEG	C4-C3-O2-C2
4	A	302	PEG	C1-C2-O2-C3
4	H	101	PEG	C1-C2-O2-C3
4	E	101	PEG	O1-C1-C2-O2
4	G	303	PEG	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	310	SO4	1	0
4	K	101	PEG	2	0
5	J	303	SO4	1	0
5	K	102	SO4	1	0
4	E	101	PEG	1	0
4	N	101	PEG	1	0
4	H	101	PEG	2	0
4	A	302	PEG	1	0
5	H	102	SO4	1	0
6	D	311	EDO	1	0
5	E	102	SO4	1	0
4	N	102	PEG	2	0
5	A	304	SO4	1	0
4	G	302	PEG	1	0
4	J	301	PEG	1	0
4	B	101	PEG	2	0
5	D	306	SO4	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	276/276 (100%)	1.09	40 (14%) 6 5	27, 59, 97, 116	0
1	D	276/276 (100%)	0.68	21 (7%) 20 17	21, 40, 65, 80	1 (0%)
1	G	276/276 (100%)	0.74	37 (13%) 7 5	19, 52, 83, 96	1 (0%)
1	J	276/276 (100%)	0.64	13 (4%) 36 32	29, 57, 93, 116	0
1	M	276/276 (100%)	0.89	32 (11%) 9 8	22, 51, 82, 104	0
2	B	100/100 (100%)	0.39	4 (4%) 42 38	22, 43, 66, 77	1 (1%)
2	E	100/100 (100%)	0.27	3 (3%) 52 48	20, 38, 59, 78	1 (1%)
2	H	100/100 (100%)	0.06	0 100 100	25, 38, 55, 67	0
2	K	100/100 (100%)	0.08	0 100 100	21, 35, 58, 75	0
2	N	100/100 (100%)	-0.12	0 100 100	13, 27, 46, 60	1 (1%)
3	C	10/10 (100%)	2.13	5 (50%) 0 0	71, 81, 90, 93	0
3	F	10/10 (100%)	0.43	0 100 100	38, 41, 46, 51	0
3	I	10/10 (100%)	0.28	0 100 100	40, 43, 47, 52	0
3	L	10/10 (100%)	1.08	1 (10%) 12 10	47, 56, 63, 69	0
3	O	10/10 (100%)	1.47	2 (20%) 3 2	49, 64, 71, 77	0
All	All	1930/1930 (100%)	0.64	158 (8%) 17 15	13, 46, 86, 116	5 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	GLY	4.9
1	M	158	ALA	4.9
1	M	149	ALA	4.4
1	G	251	SER	4.2
1	G	228	THR	4.0
1	J	193	ALA	4.0
3	C	8	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	3.8
1	G	104	GLY	3.7
1	G	194	VAL	3.6
1	G	230	LEU	3.6
1	A	41	ALA	3.6
1	A	110	LEU	3.6
1	J	276	PRO	3.5
1	A	112	GLY	3.5
1	A	195	SER	3.5
3	C	5	LEU	3.4
1	M	193	ALA	3.4
1	G	264	GLU	3.3
1	A	165	VAL	3.3
1	A	149	ALA	3.3
3	L	8	PHE	3.3
1	A	1	GLY	3.3
1	G	1	GLY	3.2
1	D	224	GLN	3.2
1	G	274	TRP	3.2
1	A	169	ARG	3.1
1	M	130	LEU	3.1
1	A	158	ALA	3.1
2	E	0	MET	3.1
1	D	226	GLN	3.0
3	O	8	PHE	3.0
1	A	104	GLY	3.0
1	D	180	GLN	3.0
1	G	255	GLN	3.0
3	O	4	ALA	3.0
1	A	105	SER	3.0
1	D	228	THR	3.0
1	D	225	THR	2.9
1	D	153	ALA	2.9
1	A	109	PHE	2.9
1	G	195	SER	2.9
1	A	193	ALA	2.9
1	G	181	ARG	2.8
1	M	1	GLY	2.8
1	A	57	PRO	2.8
1	D	227	ASP	2.8
1	M	72	GLN	2.8
1	M	268	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	276	PRO	2.8
1	G	178	THR	2.8
1	M	145	HIS	2.8
1	G	259	CYS	2.8
1	J	104	GLY	2.7
1	D	274	TRP	2.7
1	G	247	VAL	2.7
1	A	172	LEU	2.7
1	A	176	LYS	2.7
1	J	194	VAL	2.7
1	G	246	ALA	2.7
1	A	145	HIS	2.7
1	G	182	THR	2.7
1	G	268	LYS	2.6
1	A	113	TYR	2.6
1	M	109	PHE	2.6
1	M	125	ALA	2.6
1	G	217	TRP	2.6
1	G	252	GLY	2.6
1	G	249	VAL	2.6
1	D	221	GLY	2.5
1	D	230	LEU	2.5
1	D	215	LEU	2.5
3	C	4	ALA	2.5
1	M	267	PRO	2.5
1	A	108	ARG	2.5
1	M	143	THR	2.5
2	B	73	THR	2.5
1	A	156	LEU	2.5
1	A	163	THR	2.5
2	B	77	GLU	2.4
1	M	102	ASP	2.4
1	A	153	ALA	2.4
1	M	228	THR	2.4
1	G	269	PRO	2.4
1	G	276	PRO	2.4
1	M	164	CYS	2.4
1	A	179	LEU	2.4
1	G	209	TYR	2.4
1	D	205	ALA	2.4
1	G	271	THR	2.4
1	A	102	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	248	VAL	2.4
1	D	196	ASP	2.4
1	D	223	ASP	2.4
1	M	126	LEU	2.4
1	G	254	GLU	2.4
1	J	166	GLU	2.4
1	J	226	GLN	2.3
1	M	152	VAL	2.3
1	J	225	THR	2.3
1	M	3	HIS	2.3
1	M	132	SER	2.3
1	G	272	LEU	2.3
1	G	177	GLU	2.3
1	D	178	THR	2.3
1	J	182	THR	2.3
1	M	151	HIS	2.3
3	C	6	GLY	2.3
1	J	105	SER	2.3
2	B	75	LYS	2.3
1	G	257	TYR	2.3
1	D	232	GLU	2.2
1	J	57	PRO	2.2
1	A	178	THR	2.2
1	D	173	GLU	2.2
1	A	111	ARG	2.2
1	A	192	HIS	2.2
1	M	196	ASP	2.2
1	A	60	TRP	2.2
1	A	181	ARG	2.2
2	B	81[A]	ARG	2.2
1	G	265	GLY	2.2
1	A	132	SER	2.2
1	A	107	TRP	2.2
1	A	267	PRO	2.2
1	G	224	GLN	2.1
1	A	266	LEU	2.1
1	D	17	ARG	2.1
1	M	264	GLU	2.1
1	G	267	PRO	2.1
1	J	248	VAL	2.1
1	A	162	GLY	2.1
1	M	159	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	226	GLN	2.1
1	A	154	GLU	2.1
1	J	275	GLU	2.1
3	C	7	ILE	2.1
1	D	105	SER	2.1
1	G	203	CYS	2.1
1	M	269	PRO	2.1
1	M	197	HIS	2.1
1	A	167	TRP	2.1
1	M	266	LEU	2.1
2	E	1	ILE	2.1
1	A	268	LYS	2.1
1	G	196	ASP	2.1
1	D	276	PRO	2.1
1	M	153	ALA	2.0
2	E	3[A]	ARG	2.0
1	A	130	LEU	2.0
1	M	110	LEU	2.0
1	M	113	TYR	2.0
1	A	36	PHE	2.0
1	G	275	GLU	2.0
1	J	110	LEU	2.0
1	M	56	GLY	2.0
1	M	127	LYS	2.0
1	G	210	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	SO4	D	308	5/5	0.47	0.21	116,117,125,126	0
5	SO4	D	305	5/5	0.52	0.19	48,49,53,56	5
5	SO4	J	303	5/5	0.52	0.14	97,98,107,113	0
5	SO4	A	303	5/5	0.56	0.16	83,95,104,108	0
6	EDO	D	311	4/4	0.56	0.30	66,67,68,70	0
5	SO4	K	103	5/5	0.58	0.16	106,115,122,125	0
5	SO4	G	306	5/5	0.58	0.21	121,122,125,125	0
5	SO4	A	304	5/5	0.61	0.23	151,151,162,173	0
5	SO4	G	307	5/5	0.62	0.20	105,107,108,110	0
5	SO4	G	305	5/5	0.63	0.19	108,117,117,120	0
4	PEG	G	302	7/7	0.64	0.22	64,73,79,82	0
5	SO4	D	309	5/5	0.64	0.22	100,106,109,111	0
5	SO4	D	307	5/5	0.65	0.14	98,99,107,108	0
5	SO4	E	103	5/5	0.70	0.33	102,103,118,126	0
4	PEG	G	303	7/7	0.74	0.22	61,77,90,95	0
5	SO4	K	102	5/5	0.78	0.27	28,31,35,36	5
4	PEG	J	301	7/7	0.79	0.18	56,62,66,67	0
5	SO4	D	306	5/5	0.80	0.13	111,111,113,114	5
4	PEG	H	101	7/7	0.80	0.21	52,57,61,61	0
4	PEG	D	303	7/7	0.80	0.22	50,65,76,77	0
4	PEG	E	101	7/7	0.80	0.21	57,68,71,72	0
4	PEG	A	302	7/7	0.80	0.18	55,57,60,63	0
4	PEG	D	301	7/7	0.80	0.20	39,45,56,56	0
4	PEG	A	301	7/7	0.81	0.17	39,42,52,53	0
5	SO4	E	102	5/5	0.81	0.24	23,24,26,26	5
5	SO4	D	304	5/5	0.81	0.12	83,83,88,89	0
5	SO4	J	302	5/5	0.81	0.19	72,74,78,84	0
5	SO4	G	304	5/5	0.82	0.19	79,81,83,84	0
4	PEG	G	301	7/7	0.82	0.21	42,53,62,66	0
5	SO4	N	103	5/5	0.82	0.23	57,57,70,74	0
4	PEG	K	101	7/7	0.82	0.23	43,50,56,57	0
4	PEG	B	101	7/7	0.84	0.33	38,42,47,47	0
4	PEG	N	102	7/7	0.84	0.27	42,47,47,47	0
5	SO4	D	310	5/5	0.84	0.23	144,144,146,150	0
4	PEG	D	302	7/7	0.87	0.15	49,53,58,59	0
6	EDO	B	102	4/4	0.88	0.17	31,33,34,34	0
5	SO4	H	102	5/5	0.88	0.19	18,18,20,20	5
6	EDO	M	301	4/4	0.88	0.15	52,55,55,57	0
4	PEG	N	101	7/7	0.92	0.16	39,39,41,44	0
6	EDO	N	104	4/4	0.94	0.10	33,34,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.