



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:04 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 wwPDB X-ray Structure Validation Summary 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

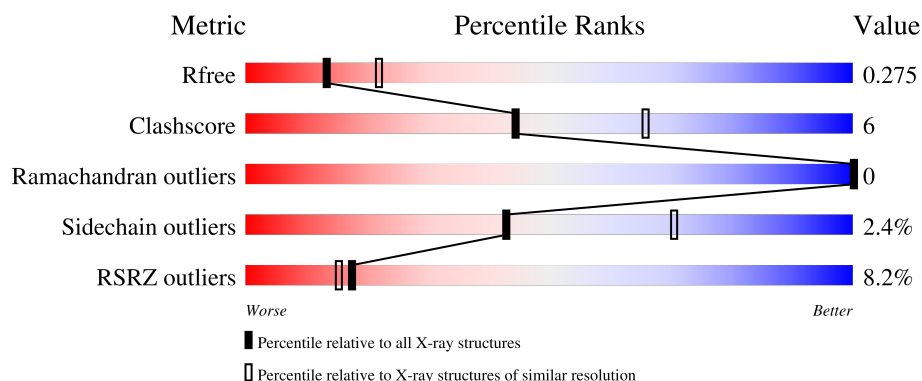
1 Overall quality at a glance

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%

Continued on next page...

Continued from previous page...

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			

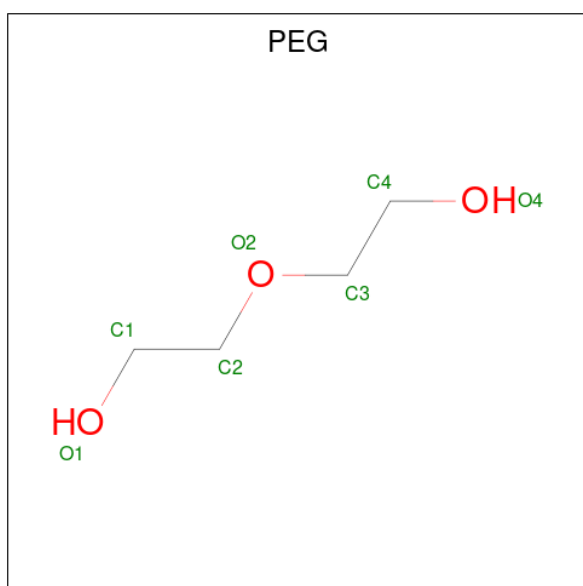
There are 5 discrepancies between the modelled and reference sequences:

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

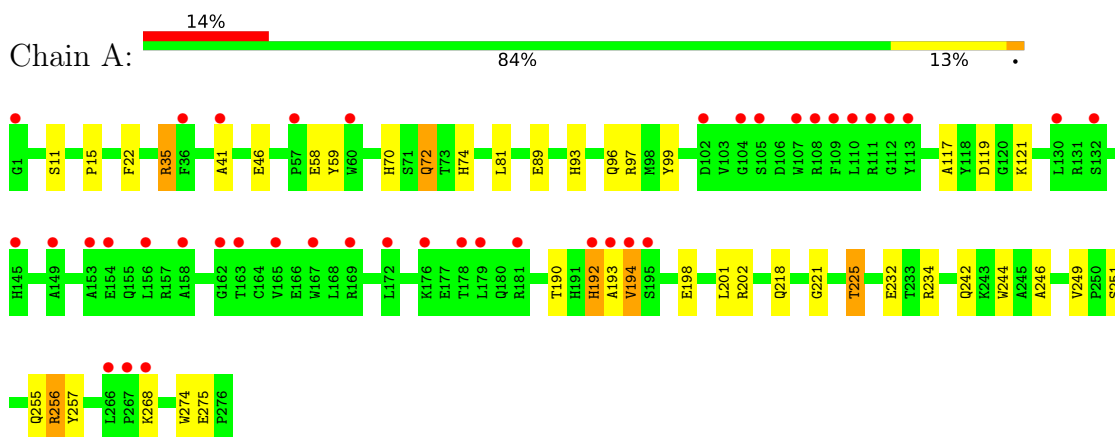
Continued from previous page...

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

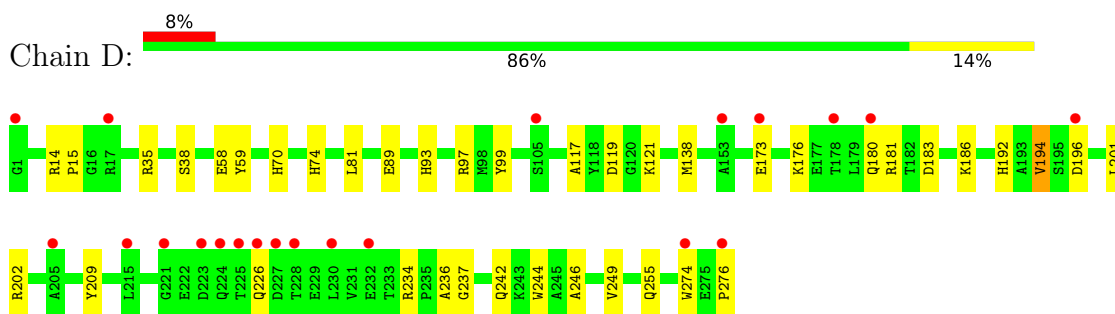
3 Residue-property plots [i](#)

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.

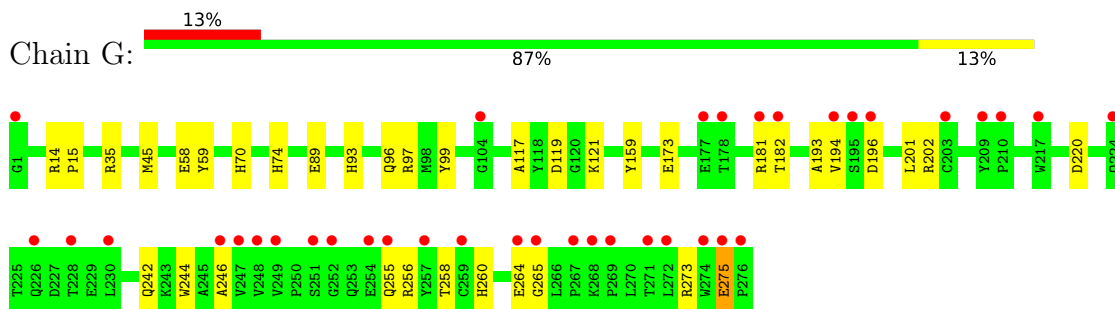
- Molecule 1: MHC class I antigen



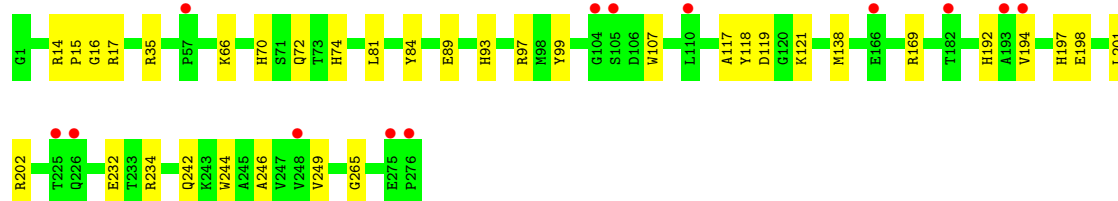
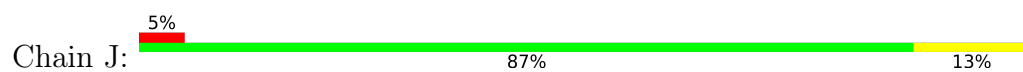
- Molecule 1: MHC class I antigen



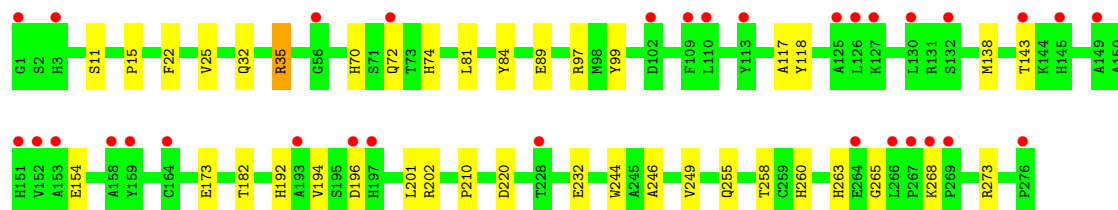
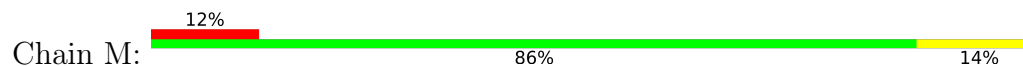
- Molecule 1: MHC class I antigen



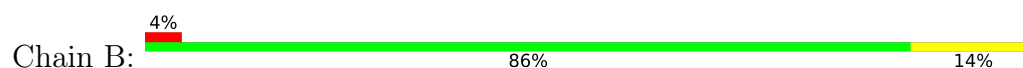
- Molecule 1: MHC class I antigen



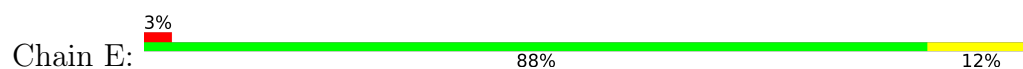
- Molecule 1: MHC class I antigen



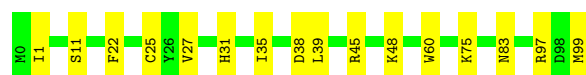
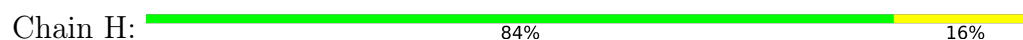
- Molecule 2: Beta-2-microglobulin



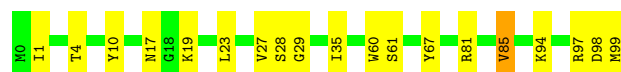
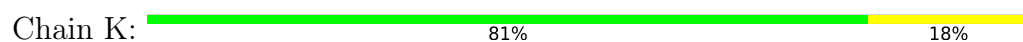
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

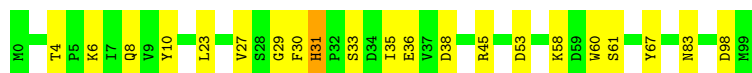


- Molecule 2: Beta-2-microglobulin



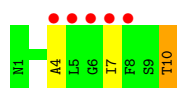
- Molecule 2: Beta-2-microglobulin

Chain N:  79% 20% .



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

Chain C:  50% 70% 20% 10%



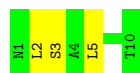
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain F:  90% 10%



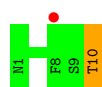
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

Chain I:  70% 30%



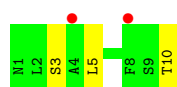
- Molecule 3: ASN-LEU-SER-ALA-LEU-GLY-ILE-PHE-SER-THR

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 [i](#)

5.1 Standard geometry [i](#)

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

The worst 5 of 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

Continued on next page...

Continued from previous page...

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

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	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
5	A	10	0	0	1	0
5	D	35	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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
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

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	72	GLN
1	M	194	VAL
1	J	194	VAL
3	L	10	THR
1	M	249	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	86	ASN
1	M	180	GLN
1	M	263	HIS
1	D	242	GLN
1	D	192	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	G	302	-	-	3/4/4/4	-
4	PEG	D	301	-	-	1/4/4/4	-
4	PEG	J	301	-	-	2/4/4/4	-
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.

5 of 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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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%)

The worst 5 of 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

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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.