



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:35 AM UTC

PDB ID : 3Q3G / pdb_00003q3g
Title : Crystal Structure of A-domain in complex with antibody
Authors : Mahalingam, B.; Xiong, J.P.; Arnaout, M.A.
Deposited on : 2010-12-21
Resolution : 2.70 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

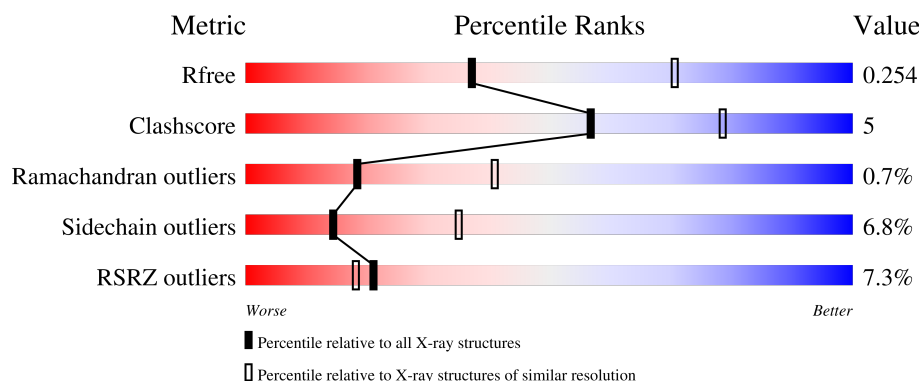
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	220	% 80%18%.
1	C	220	3% 81%18%.
1	F	220	20% 83%15%.
1	J	220	% 80%16%.
2	B	224	2% 83%15%.

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Mol	Chain	Length	Quality of chain
2	D	224	2%83%16%
2	H	224	2%83%15%
2	K	224	2%86%14%
3	E	190	2%83%15%
3	G	190	2%80%18%
3	I	190	32%80%18%
3	L	190	23%79%16%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20257 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 Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	A	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	F	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			
1	J	220	Total	C	N	O	S	0	0	0
			1718	1074	283	353	8			

- Molecule 2 is a protein called Antibody Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	B	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	H	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			
2	K	224	Total	C	N	O	S	0	0	0
			1689	1062	277	342	8			

- Molecule 3 is a protein called Integrin alpha-M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	189	Total	C	N	O	S	0	0	0
			1531	975	271	282	3			
3	E	189	Total	C	N	O	S	0	0	0
			1531	975	271	282	3			
3	I	189	Total	C	N	O	S	0	0	0
			1531	975	271	282	3			
3	L	189	Total	C	N	O	S	0	0	0
			1531	975	271	282	3			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



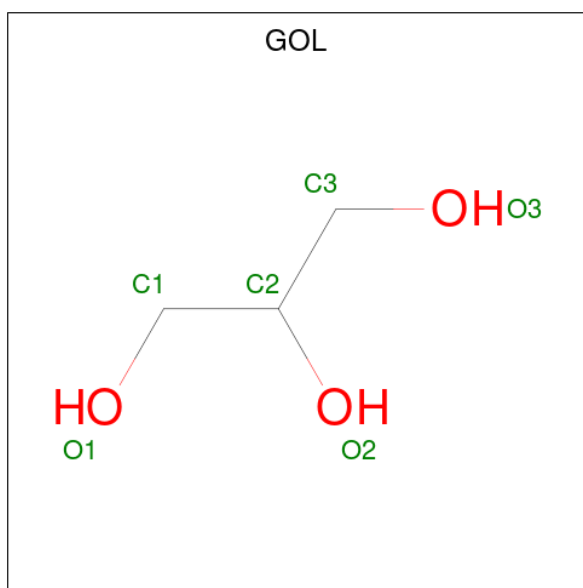
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0
6	H	2	Total Na 2 2	0	0

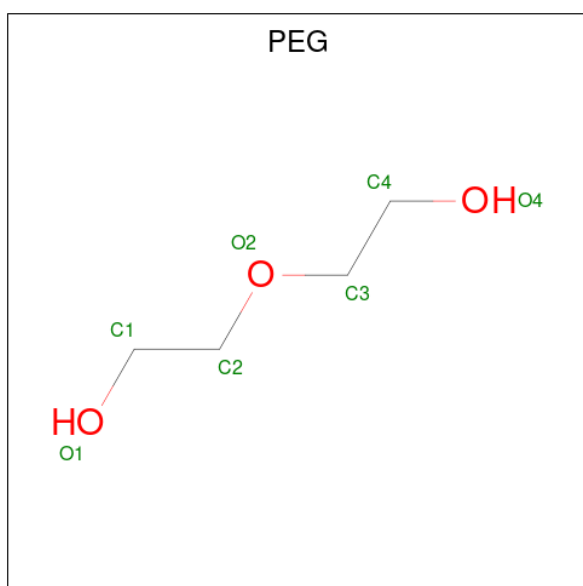
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0
7	I	1	Total Ca 1 1	0	0
7	L	1	Total Ca 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	1	Total Cl 1 1	0	0
8	E	2	Total Cl 2 2	0	0
8	J	1	Total Cl 1 1	0	0
8	K	1	Total Cl 1 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C O 7 4 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	42	Total O 42 42	0	0
10	D	42	Total O 42 42	0	0
10	G	29	Total O 29 29	0	0
10	A	31	Total O 31 31	0	0
10	B	49	Total O 49 49	0	0

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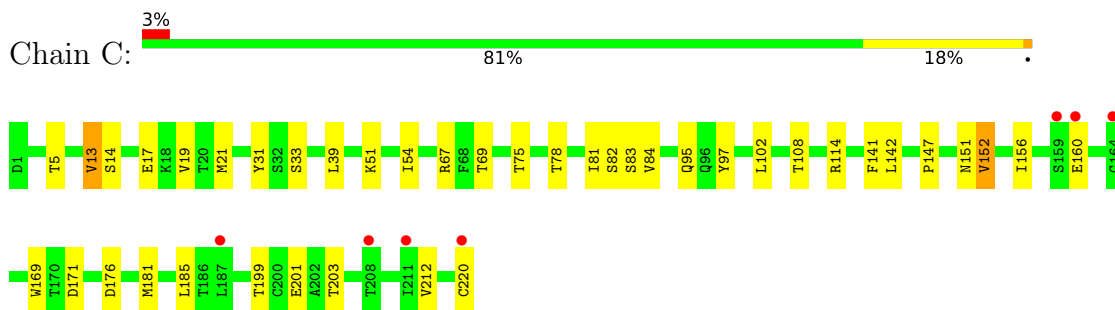
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	E	12	Total 12	O 12	0	0
10	F	6	Total 6	O 6	0	0
10	H	22	Total 22	O 22	0	0
10	I	6	Total 6	O 6	0	0
10	J	31	Total 31	O 31	0	0
10	K	40	Total 40	O 40	0	0
10	L	10	Total 10	O 10	0	0

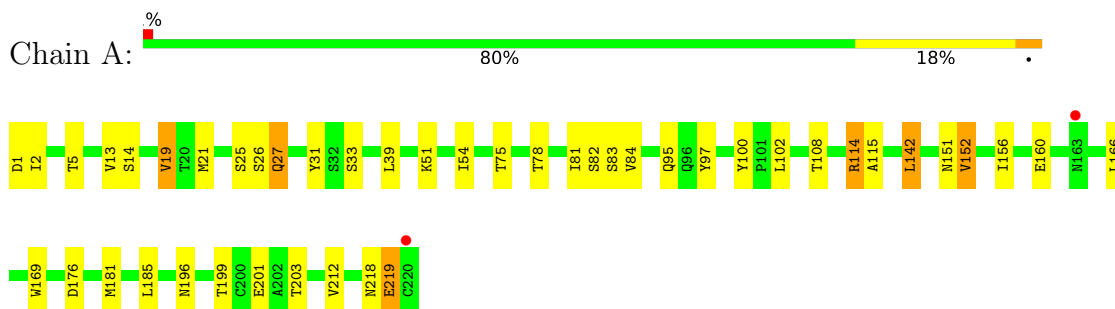
3 Residue-property plots [i](#)

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.

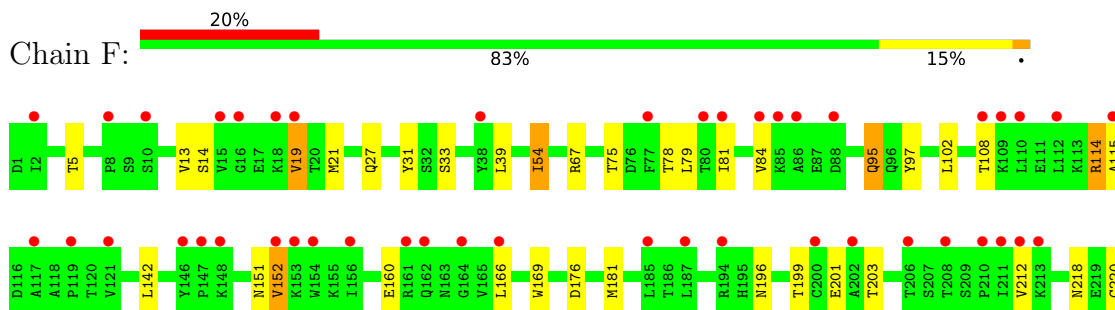
• Molecule 1: Antibody Light Chain



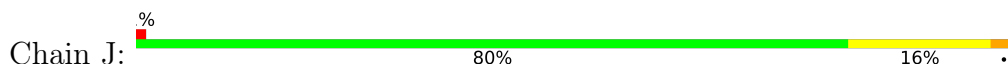
• Molecule 1: Antibody Light Chain

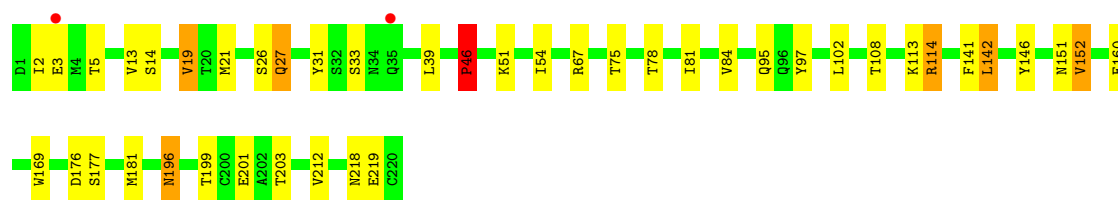


• Molecule 1: Antibody Light Chain

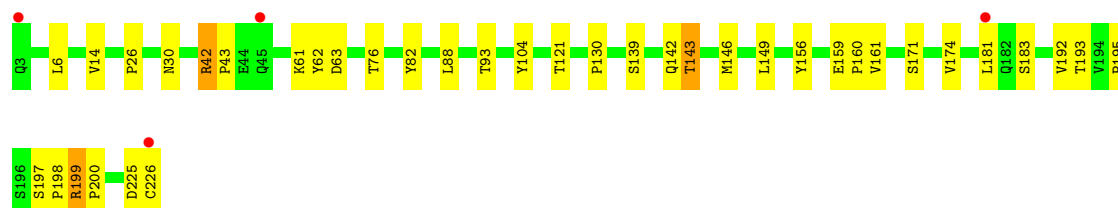
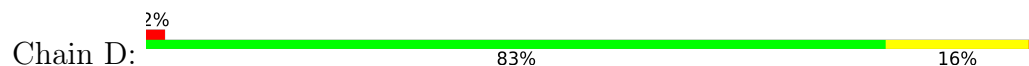


• Molecule 1: Antibody Light Chain

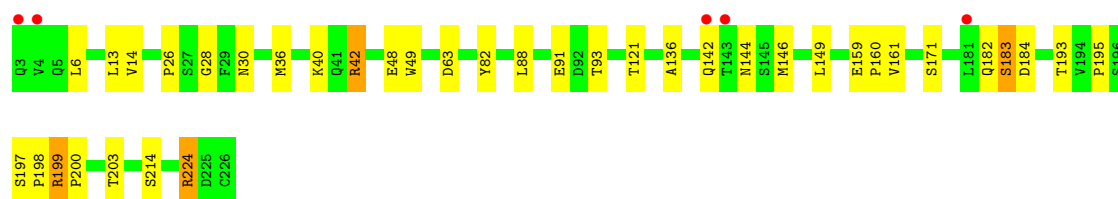
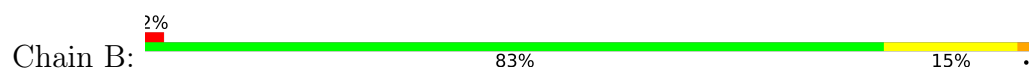




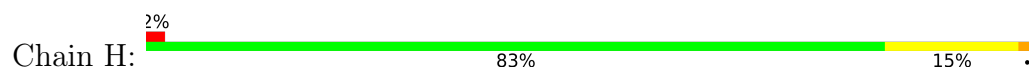
• Molecule 2: Antibody Heavy chain



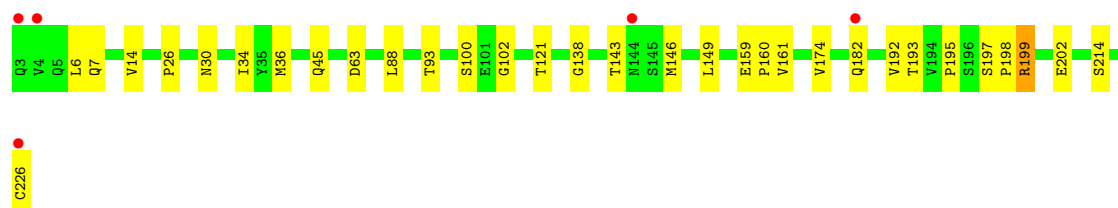
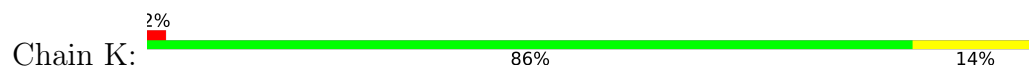
• Molecule 2: Antibody Heavy chain



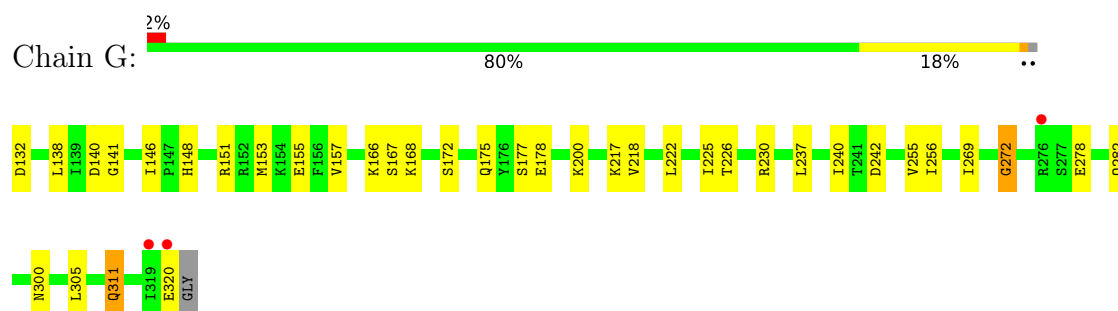
• Molecule 2: Antibody Heavy chain



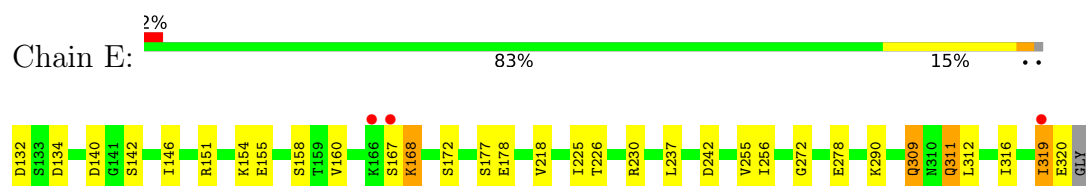
• Molecule 2: Antibody Heavy chain



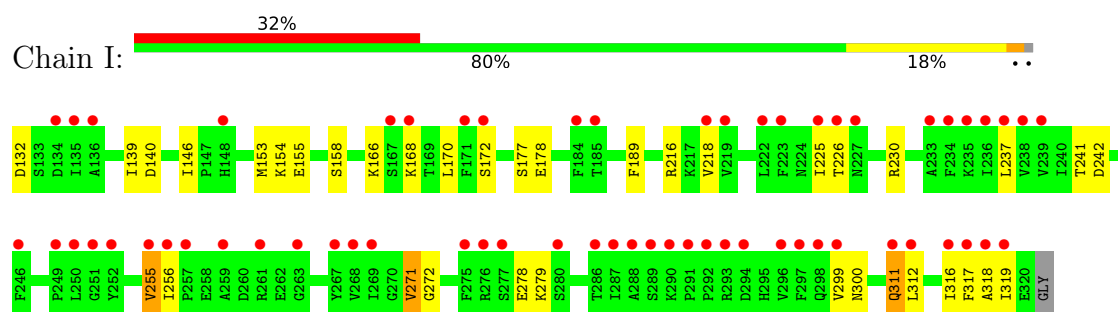
- Molecule 3: Integrin alpha-M



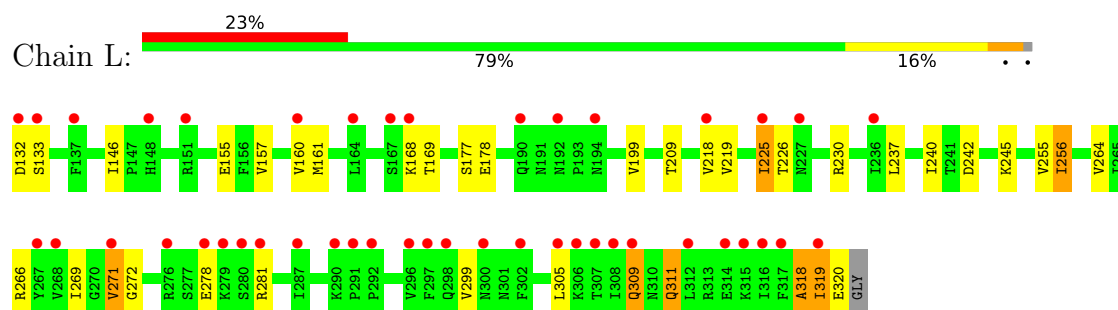
- Molecule 3: Integrin alpha-M



- Molecule 3: Integrin alpha-M



- Molecule 3: Integrin alpha-M



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.94Å 157.22Å 232.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.76 – 2.70 47.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (47.76-2.70) 97.2 (47.76-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.211 , 0.244 0.221 , 0.254	Depositor DCC
R_{free} test set	4053 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20257	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, NA, EDO, CA, CL, GOL

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	0.74	0/1757	1.18	4/2384 (0.2%)
1	C	0.73	0/1757	1.17	5/2384 (0.2%)
1	F	0.68	0/1757	1.14	1/2384 (0.0%)
1	J	0.72	0/1757	1.19	6/2384 (0.3%)
2	B	0.73	0/1732	1.20	4/2368 (0.2%)
2	D	0.76	0/1732	1.22	5/2368 (0.2%)
2	H	0.74	0/1732	1.19	2/2368 (0.1%)
2	K	0.75	0/1732	1.19	3/2368 (0.1%)
3	E	0.79	1/1560 (0.1%)	1.42	16/2099 (0.8%)
3	G	0.83	1/1560 (0.1%)	1.42	11/2099 (0.5%)
3	I	0.82	1/1560 (0.1%)	1.40	12/2099 (0.6%)
3	L	0.84	1/1560 (0.1%)	1.43	9/2099 (0.4%)
All	All	0.76	4/20196 (0.0%)	1.26	78/27404 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	256	ILE	CA-CB	7.66	1.58	1.54
3	I	256	ILE	CA-CB	6.45	1.57	1.54
3	E	256	ILE	CA-CB	5.12	1.56	1.54
3	G	256	ILE	CA-CB	5.02	1.57	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	255	VAL	CA-C-N	7.84	126.61	120.33
3	L	255	VAL	C-N-CA	7.84	126.61	120.33
1	A	219	GLU	CA-C-N	7.65	135.47	121.70
1	A	219	GLU	C-N-CA	7.65	135.47	121.70
3	E	140	ASP	CA-CB-CG	7.42	120.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	167	SER	N-CA-C	-7.24	96.76	108.41
3	G	140	ASP	CA-CB-CG	7.18	119.78	112.60
2	K	63	ASP	N-CA-C	-7.13	100.81	109.72
2	B	63	ASP	N-CA-C	-7.10	100.85	109.72
2	B	144	ASN	CA-CB-CG	7.09	119.69	112.60
2	H	63	ASP	N-CA-C	-6.96	101.02	109.72
2	D	63	ASP	N-CA-C	-6.80	101.22	109.72
3	G	255	VAL	CA-C-N	6.71	125.70	120.33
3	G	255	VAL	C-N-CA	6.71	125.70	120.33
3	L	318	ALA	CA-C-N	6.67	133.70	121.70
3	L	318	ALA	C-N-CA	6.67	133.70	121.70
3	I	272	GLY	CA-C-N	6.58	131.22	120.63
3	I	272	GLY	C-N-CA	6.58	131.22	120.63
3	L	272	GLY	CA-C-N	6.42	129.76	120.38
3	L	272	GLY	C-N-CA	6.42	129.76	120.38
3	E	272	GLY	CA-C-N	6.41	129.74	120.38
3	E	272	GLY	C-N-CA	6.41	129.74	120.38
3	I	178	GLU	N-CA-C	-6.37	105.44	113.72
3	G	178	GLU	N-CA-C	-6.32	105.50	113.72
3	E	178	GLU	N-CA-C	-6.25	105.60	113.72
3	E	167	SER	CA-C-N	6.19	133.36	121.54
3	E	167	SER	C-N-CA	6.19	133.36	121.54
1	J	219	GLU	CA-C-N	6.17	132.81	121.70
1	J	219	GLU	C-N-CA	6.17	132.81	121.70
3	L	178	GLU	N-CA-C	-6.17	105.70	113.72
3	I	255	VAL	CA-C-N	6.13	125.24	120.33
3	I	255	VAL	C-N-CA	6.13	125.24	120.33
3	I	154	LYS	CA-C-N	6.09	128.35	120.44
3	I	154	LYS	C-N-CA	6.09	128.35	120.44
1	J	46	PRO	CB-CA-C	6.08	121.59	111.56
3	E	134	ASP	CA-CB-CG	5.87	118.47	112.60
1	J	46	PRO	N-CA-C	5.79	124.41	112.47
3	G	255	VAL	N-CA-CB	-5.78	106.90	111.64
2	D	181	LEU	CA-C-N	5.72	131.23	123.11
2	D	181	LEU	C-N-CA	5.72	131.23	123.11
3	E	255	VAL	N-CA-CB	-5.70	106.97	111.64
1	A	176	ASP	CA-CB-CG	5.54	118.14	112.60
3	I	255	VAL	N-CA-C	5.50	116.74	112.12
2	H	91	GLU	CB-CG-CD	5.47	121.90	112.60
1	J	176	ASP	CA-CB-CG	5.42	118.02	112.60
3	G	305	LEU	CA-C-N	5.41	128.28	120.38
3	G	305	LEU	C-N-CA	5.41	128.28	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	91	GLU	CB-CG-CD	5.37	121.72	112.60
3	G	272	GLY	CA-C-N	5.34	129.22	120.63
3	G	272	GLY	C-N-CA	5.34	129.22	120.63
3	I	278	GLU	CA-C-N	5.34	127.43	120.28
3	I	278	GLU	C-N-CA	5.34	127.43	120.28
1	C	141	PHE	CA-CB-CG	5.32	119.12	113.80
2	B	203	THR	N-CA-C	5.30	117.39	108.96
1	F	176	ASP	CA-CB-CG	5.30	117.90	112.60
3	E	154	LYS	CA-C-N	5.30	127.81	120.29
3	E	154	LYS	C-N-CA	5.30	127.81	120.29
2	K	138	GLY	CA-C-N	5.28	127.62	120.38
2	K	138	GLY	C-N-CA	5.28	127.62	120.38
3	L	255	VAL	N-CA-C	5.25	115.77	111.62
3	L	271	VAL	N-CA-C	5.19	115.57	107.99
1	A	82	SER	N-CA-C	-5.19	102.00	110.20
1	C	171	ASP	CA-CB-CG	5.18	117.78	112.60
2	D	143	THR	CA-C-N	5.17	128.56	120.75
2	D	143	THR	C-N-CA	5.17	128.56	120.75
3	G	167	SER	N-CA-C	5.17	118.68	112.38
3	G	255	VAL	N-CA-C	5.15	115.69	111.62
3	E	319	ILE	CA-C-N	5.12	130.91	121.70
3	E	319	ILE	C-N-CA	5.12	130.91	121.70
3	I	318	ALA	CA-C-N	5.12	131.18	121.97
3	I	318	ALA	C-N-CA	5.12	131.18	121.97
1	C	176	ASP	CA-CB-CG	5.11	117.71	112.60
1	J	141	PHE	CA-CB-CG	5.04	118.84	113.80
3	E	142	SER	CA-C-N	5.03	126.47	120.13
3	E	142	SER	C-N-CA	5.03	126.47	120.13
3	E	319	ILE	CB-CA-C	5.03	119.54	111.29
1	C	147	PRO	CA-C-N	5.01	127.70	120.38
1	C	147	PRO	C-N-CA	5.01	127.70	120.38

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	1718	0	1647	14	0
1	C	1718	0	1647	14	0
1	F	1718	0	1647	13	0
1	J	1718	0	1647	12	0
2	B	1689	0	1638	23	0
2	D	1689	0	1638	22	0
2	H	1689	0	1638	22	0
2	K	1689	0	1638	19	0
3	E	1531	0	1545	6	0
3	G	1531	0	1545	14	0
3	I	1531	0	1545	11	0
3	L	1531	0	1545	17	0
4	A	8	0	12	0	0
4	B	16	0	24	3	0
4	C	8	0	12	0	0
4	D	20	0	30	3	0
4	E	8	0	12	1	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	J	8	0	12	0	0
4	K	16	0	24	0	0
4	L	8	0	12	0	0
5	A	6	0	8	1	0
5	B	12	0	16	1	0
5	C	6	0	8	0	0
5	D	18	0	24	1	0
5	G	6	0	8	1	0
5	J	6	0	8	0	0
5	K	12	0	16	1	0
6	D	1	0	0	0	0
6	H	2	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	I	1	0	0	0	0
7	L	1	0	0	0	0
8	E	2	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
8	K	1	0	0	0	0
9	H	7	0	10	0	0
10	A	31	0	0	0	0
10	B	49	0	0	0	0
10	C	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	42	0	0	0	0
10	E	12	0	0	0	0
10	F	6	0	0	1	0
10	G	29	0	0	0	0
10	H	22	0	0	0	0
10	I	6	0	0	0	0
10	J	31	0	0	0	0
10	K	40	0	0	0	0
10	L	10	0	0	1	0
All	All	20257	0	19568	180	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 5.

All (180) 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:B:199:ARG:HG3	2:B:199:ARG:HH11	1.00	1.12
2:D:199:ARG:HH11	2:D:199:ARG:HG3	1.09	1.10
1:C:13:VAL:HG22	1:C:19:VAL:HG11	1.41	1.02
2:K:199:ARG:HH11	2:K:199:ARG:HG3	1.23	1.00
2:H:199:ARG:HG2	2:H:200:PRO:HA	1.43	0.97
2:B:199:ARG:HH11	2:B:199:ARG:CG	1.86	0.89
2:D:199:ARG:HG3	2:D:199:ARG:NH1	1.89	0.87
2:B:199:ARG:HG3	2:B:199:ARG:NH1	1.80	0.87
1:C:13:VAL:CG2	1:C:19:VAL:HG11	2.05	0.86
2:K:199:ARG:HH11	2:K:199:ARG:CG	1.88	0.85
2:H:149:LEU:HD11	2:H:199:ARG:HD3	1.62	0.81
5:D:702:GOL:H12	2:H:202:GLU:OE1	1.83	0.78
2:D:199:ARG:HH11	2:D:199:ARG:CG	1.93	0.77
1:C:21:MET:HG2	1:C:108:THR:HG21	1.67	0.77
1:F:21:MET:HG2	1:F:108:THR:HG21	1.70	0.73
1:F:142:LEU:HD11	1:F:152:VAL:HG13	1.70	0.73
1:A:142:LEU:HD11	1:A:152:VAL:HG13	1.70	0.73
2:K:199:ARG:HG3	2:K:199:ARG:NH1	1.97	0.72
1:C:142:LEU:HD11	1:C:152:VAL:HG13	1.70	0.72
1:C:201:GLU:HG3	1:C:212:VAL:HG22	1.73	0.71
1:J:142:LEU:HD11	1:J:152:VAL:HG13	1.72	0.70
1:A:201:GLU:HG3	1:A:212:VAL:HG22	1.73	0.70
1:J:201:GLU:HG3	1:J:212:VAL:HG22	1.73	0.70
1:F:54:ILE:HD13	1:F:79:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:GLU:HG3	1:F:212:VAL:HG22	1.73	0.69
1:J:19:VAL:HG13	1:J:81:ILE:HB	1.76	0.67
2:B:195:PRO:HB2	2:B:198:PRO:HD2	1.77	0.66
2:H:34:ILE:HG22	2:H:102:GLY:HA2	1.76	0.66
2:H:195:PRO:HB2	2:H:198:PRO:HD2	1.77	0.66
2:D:195:PRO:HB2	2:D:198:PRO:HD2	1.78	0.66
1:J:21:MET:HG2	1:J:108:THR:HG21	1.78	0.65
1:A:100:TYR:HB2	4:E:600:EDO:H21	1.78	0.65
2:K:195:PRO:HB2	2:K:198:PRO:HD2	1.80	0.64
3:L:271:VAL:HG13	3:L:299:VAL:HG23	1.83	0.61
2:H:42:ARG:O	2:H:44:GLU:HA	2.00	0.61
2:D:149:LEU:HD11	2:D:199:ARG:HG2	1.82	0.61
1:F:169:TRP:CD1	1:F:181:MET:HG3	2.36	0.61
3:G:218:VAL:HG11	3:G:237:LEU:HD13	1.83	0.60
1:F:166:LEU:HD21	2:H:182:GLN:HE21	1.65	0.60
2:B:149:LEU:HD11	2:B:199:ARG:HG2	1.84	0.60
1:A:169:TRP:CD1	1:A:181:MET:HG3	2.36	0.60
1:C:169:TRP:CD1	1:C:181:MET:HG3	2.36	0.59
1:J:196:ASN:HD21	1:J:218:ASN:HB2	1.67	0.59
3:I:218:VAL:HG11	3:I:237:LEU:HD13	1.85	0.59
3:L:318:ALA:HB1	3:L:319:ILE:HG23	1.85	0.59
3:L:225:ILE:HD12	10:L:1098:HOH:O	2.02	0.58
1:J:169:TRP:CD1	1:J:181:MET:HG3	2.37	0.58
1:J:113:LYS:HA	1:J:146:TYR:OH	2.04	0.58
1:A:19:VAL:HG13	1:A:81:ILE:HB	1.84	0.58
1:A:21:MET:HG2	1:A:108:THR:HG21	1.84	0.57
2:K:199:ARG:CG	2:K:199:ARG:NH1	2.58	0.57
1:A:156:ILE:HD11	1:A:185:LEU:HD21	1.86	0.57
3:E:218:VAL:HG11	3:E:237:LEU:HD13	1.86	0.57
3:I:139:ILE:HB	3:I:153:MET:HE3	1.86	0.56
3:I:271:VAL:HG13	3:I:299:VAL:HG23	1.86	0.56
3:L:278:GLU:HG3	3:L:281:ARG:HH11	1.70	0.56
3:L:218:VAL:HG11	3:L:237:LEU:HD13	1.87	0.56
3:L:157:VAL:HG12	3:L:161:MET:HE2	1.87	0.55
2:K:14:VAL:HG21	2:K:88:LEU:HD13	1.89	0.55
2:B:40:LYS:HE2	2:B:42:ARG:HD2	1.88	0.55
2:B:48:GLU:HA	4:B:607:EDO:H21	1.88	0.55
3:L:269:ILE:HG21	3:L:305:LEU:HD11	1.89	0.55
3:E:311:GLN:HE21	3:E:311:GLN:H	1.55	0.54
3:G:166:LYS:NZ	3:G:320:GLU:HG2	2.22	0.54
3:G:311:GLN:HE21	3:G:311:GLN:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:TYR:CZ	1:J:33:SER:HB2	2.43	0.54
3:G:148:HIS:HD2	3:G:151:ARG:NH2	2.04	0.54
1:J:114:ARG:HG2	1:J:177:SER:HB2	1.90	0.54
2:B:214:SER:HA	5:B:704:GOL:H2	1.89	0.54
2:H:159:GLU:HG3	2:H:160:PRO:HA	1.90	0.54
2:B:159:GLU:HG3	2:B:160:PRO:HA	1.90	0.54
2:B:199:ARG:CG	2:B:199:ARG:NH1	2.55	0.53
2:D:174:VAL:HG22	2:D:192:VAL:HG23	1.90	0.53
2:K:159:GLU:HG3	2:K:160:PRO:HA	1.91	0.53
1:F:31:TYR:CZ	1:F:33:SER:HB2	2.43	0.53
3:L:160:VAL:HG23	3:L:309:GLN:HE21	1.74	0.53
2:D:199:ARG:NH1	2:D:199:ARG:CG	2.60	0.53
2:D:159:GLU:HG3	2:D:160:PRO:HA	1.92	0.52
2:H:220:LYS:HB3	2:K:214:SER:HB3	1.90	0.52
2:B:14:VAL:HG21	2:B:88:LEU:HD13	1.91	0.52
1:C:31:TYR:CZ	1:C:33:SER:HB2	2.45	0.52
3:G:240:ILE:HG12	3:G:269:ILE:HD12	1.92	0.52
2:K:149:LEU:HD11	2:K:199:ARG:HG2	1.92	0.52
3:L:311:GLN:HE21	3:L:311:GLN:H	1.56	0.52
3:I:311:GLN:HE21	3:I:311:GLN:H	1.55	0.52
3:I:170:LEU:HD13	3:I:189:PHE:HD2	1.74	0.52
1:A:31:TYR:CZ	1:A:33:SER:HB2	2.44	0.51
1:F:19:VAL:HG13	1:F:81:ILE:HB	1.92	0.51
2:H:142:GLN:HE21	2:H:144:ASN:HD21	1.58	0.51
2:D:14:VAL:HG21	2:D:88:LEU:HD13	1.91	0.51
2:D:146:MET:HE3	2:D:193:THR:HG22	1.92	0.51
1:C:17:GLU:O	1:C:84:VAL:HG23	2.11	0.51
2:H:14:VAL:HG21	2:H:88:LEU:HD13	1.93	0.51
2:D:104:TYR:HD1	3:E:151:ARG:HH21	1.58	0.51
2:K:34:ILE:HG22	2:K:102:GLY:HA2	1.94	0.50
2:K:146:MET:HE3	2:K:193:THR:HG22	1.94	0.50
2:H:146:MET:HE3	2:H:193:THR:HG22	1.94	0.49
2:K:6:LEU:HD23	2:K:26:PRO:HB3	1.94	0.49
3:L:209:THR:HG22	3:L:245:LYS:HA	1.93	0.49
2:D:199:ARG:HD2	2:D:200:PRO:HA	1.93	0.49
2:D:62:TYR:HD1	4:D:604:EDO:H12	1.77	0.49
2:H:6:LEU:HD23	2:H:26:PRO:HB3	1.95	0.49
3:I:216:ARG:HB2	3:I:255:VAL:HG12	1.94	0.49
2:B:182:GLN:O	2:B:183:SER:HB3	2.13	0.49
2:D:6:LEU:HD23	2:D:26:PRO:HB3	1.94	0.48
2:B:199:ARG:HD2	2:B:200:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:THR:H	4:D:614:EDO:H22	1.78	0.48
3:I:166:LYS:HD2	3:I:317:PHE:HE1	1.79	0.48
2:K:7:GLN:HG3	5:K:707:GOL:H32	1.96	0.48
1:C:156:ILE:HD11	1:C:185:LEU:HD21	1.96	0.48
1:A:114:ARG:HD3	1:A:115:ALA:O	2.14	0.48
3:L:240:ILE:HG12	3:L:269:ILE:HD12	1.96	0.48
2:H:34:ILE:HD13	2:H:100:SER:HB2	1.95	0.48
2:B:146:MET:HE3	2:B:193:THR:HG22	1.97	0.47
2:B:6:LEU:HD23	2:B:26:PRO:HB3	1.95	0.47
2:B:195:PRO:HB2	2:B:198:PRO:CD	2.45	0.47
3:E:312:LEU:O	3:E:316:ILE:HG12	2.14	0.47
3:L:256:ILE:HG23	3:L:266:ARG:HH21	1.80	0.47
2:D:195:PRO:HB2	2:D:198:PRO:CD	2.45	0.47
3:G:278:GLU:O	3:G:282:GLN:HG3	2.15	0.46
2:D:82:TYR:CE1	2:H:202:GLU:HG2	2.50	0.46
2:H:142:GLN:HE21	2:H:144:ASN:ND2	2.14	0.45
1:J:97:TYR:HA	1:J:102:LEU:HD22	1.99	0.45
3:G:172:SER:OG	3:G:222:LEU:HD22	2.16	0.45
1:A:1:ASP:N	5:A:700:GOL:H2	2.31	0.45
3:I:312:LEU:O	3:I:316:ILE:HG12	2.17	0.45
1:C:97:TYR:HA	1:C:102:LEU:HD22	1.99	0.45
1:F:97:TYR:HA	1:F:102:LEU:HD22	1.99	0.45
2:H:195:PRO:HB2	2:H:198:PRO:CD	2.45	0.45
1:A:97:TYR:HA	1:A:102:LEU:HD22	1.98	0.44
2:B:49:TRP:H	4:B:607:EDO:H21	1.82	0.44
2:K:195:PRO:HB2	2:K:198:PRO:CD	2.46	0.44
1:C:69:THR:HG22	10:C:1239:HOH:O	2.18	0.44
2:D:61:LYS:HA	4:D:604:EDO:H21	2.00	0.44
3:L:133:SER:O	3:L:169:THR:HA	2.18	0.44
3:L:256:ILE:HG23	3:L:266:ARG:NH2	2.33	0.44
3:E:160:VAL:HG23	3:E:309:GLN:HE21	1.83	0.43
2:H:130:PRO:HB3	2:H:156:TYR:HB3	2.00	0.43
3:I:132:ASP:HA	3:I:168:LYS:HB3	2.00	0.43
3:G:217:LYS:NZ	5:G:703:GOL:O2	2.50	0.43
1:F:95:GLN:HE21	1:F:95:GLN:HB3	1.67	0.43
2:B:93:THR:HG23	2:B:121:THR:HA	2.01	0.43
2:K:93:THR:HG23	2:K:121:THR:HA	2.00	0.43
2:D:42:ARG:HG3	2:D:43:PRO:HD2	2.01	0.43
2:H:121:THR:HG21	2:H:186:TYR:OH	2.19	0.43
3:G:132:ASP:HA	3:G:168:LYS:HB3	2.00	0.42
2:B:49:TRP:H	4:B:607:EDO:C2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:132:ASP:HA	3:L:168:LYS:HB3	2.01	0.42
3:G:153:MET:O	3:G:157:VAL:HG23	2.20	0.42
2:K:34:ILE:HD13	2:K:100:SER:HB2	2.02	0.42
1:A:2:ILE:HG12	1:A:27:GLN:HB2	2.02	0.42
2:B:26:PRO:HG3	2:B:36:MET:HE1	2.02	0.42
2:B:82:TYR:CE1	2:K:202:GLU:HG2	2.54	0.42
2:B:136:ALA:HB3	2:B:224:ARG:HH21	1.85	0.42
2:H:93:THR:HG23	2:H:121:THR:HA	2.01	0.42
2:H:175:HIS:HB2	2:H:191:SER:HB3	2.00	0.42
1:J:67:ARG:HG3	1:J:81:ILE:HG23	2.01	0.42
2:K:26:PRO:HG3	2:K:36:MET:HE1	2.01	0.42
3:G:272:GLY:HA2	3:G:300:ASN:O	2.20	0.42
1:F:196:ASN:ND2	1:F:218:ASN:H	2.18	0.41
3:L:219:VAL:HG22	3:L:264:VAL:HG21	2.01	0.41
2:D:93:THR:HG23	2:D:121:THR:HA	2.02	0.41
3:G:138:LEU:HB2	3:G:218:VAL:HG21	2.01	0.41
1:A:196:ASN:ND2	1:A:218:ASN:H	2.18	0.41
1:C:67:ARG:HG3	1:C:81:ILE:HG23	2.03	0.41
2:D:130:PRO:HB3	2:D:156:TYR:HB3	2.01	0.41
3:I:140:ASP:HB2	3:I:241:THR:HA	2.02	0.41
3:I:311:GLN:H	3:I:311:GLN:NE2	2.18	0.41
1:F:67:ARG:HB3	10:F:3223:HOH:O	2.21	0.41
1:J:2:ILE:HG12	1:J:27:GLN:HB2	2.03	0.41
2:K:174:VAL:HG22	2:K:192:VAL:HG23	2.02	0.41
1:C:220:CYS:HB3	2:D:226:CYS:HB3	1.75	0.41
3:E:132:ASP:HA	3:E:168:LYS:HB3	2.02	0.41
1:F:114:ARG:HD3	1:F:115:ALA:O	2.20	0.41
3:G:141:GLY:HA3	3:G:175:GLN:OE1	2.21	0.41
3:G:200:LYS:HE3	2:B:28:GLY:HA2	2.02	0.41
1:A:25:SER:OG	1:A:27:GLN:O	2.35	0.41
2:H:26:PRO:HG3	2:H:36:MET:HE1	2.03	0.40
3:L:311:GLN:H	3:L:311:GLN:NE2	2.19	0.40
1:C:67:ARG:HB2	1:C:82:SER:O	2.21	0.40

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	218/220 (99%)	212 (97%)	4 (2%)	2 (1%)	14	35
1	C	218/220 (99%)	212 (97%)	5 (2%)	1 (0%)	24	48
1	F	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	J	218/220 (99%)	211 (97%)	6 (3%)	1 (0%)	24	48
2	B	222/224 (99%)	210 (95%)	10 (4%)	2 (1%)	14	35
2	D	222/224 (99%)	212 (96%)	6 (3%)	4 (2%)	6	18
2	H	222/224 (99%)	211 (95%)	10 (4%)	1 (0%)	24	48
2	K	222/224 (99%)	213 (96%)	8 (4%)	1 (0%)	24	48
3	E	187/190 (98%)	178 (95%)	7 (4%)	2 (1%)	11	29
3	G	187/190 (98%)	179 (96%)	7 (4%)	1 (0%)	24	48
3	I	187/190 (98%)	180 (96%)	5 (3%)	2 (1%)	11	29
3	L	187/190 (98%)	178 (95%)	8 (4%)	1 (0%)	24	48
All	All	2508/2536 (99%)	2407 (96%)	83 (3%)	18 (1%)	18	41

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	225	ASP
3	E	168	LYS
2	H	141	ALA
1	J	46	PRO
2	B	142	GLN
2	D	142	GLN
3	G	177	SER
1	A	219	GLU
2	B	183	SER
3	E	177	SER
3	I	177	SER
3	L	177	SER

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Mol	Chain	Res	Type
1	C	83	SER
2	D	183	SER
1	A	83	SER
2	K	182	GLN
3	I	319	ILE
2	D	143	THR

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	197/197 (100%)	176 (89%)	21 (11%)	6	16
1	C	197/197 (100%)	182 (92%)	15 (8%)	12	30
1	F	197/197 (100%)	179 (91%)	18 (9%)	9	22
1	J	197/197 (100%)	174 (88%)	23 (12%)	5	13
2	B	192/192 (100%)	183 (95%)	9 (5%)	23	51
2	D	192/192 (100%)	185 (96%)	7 (4%)	31	60
2	H	192/192 (100%)	185 (96%)	7 (4%)	31	60
2	K	192/192 (100%)	185 (96%)	7 (4%)	31	60
3	E	169/169 (100%)	155 (92%)	14 (8%)	10	26
3	G	169/169 (100%)	162 (96%)	7 (4%)	27	56
3	I	169/169 (100%)	157 (93%)	12 (7%)	13	33
3	L	169/169 (100%)	158 (94%)	11 (6%)	15	37
All	All	2232/2232 (100%)	2081 (93%)	151 (7%)	14	35

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	THR
1	C	13	VAL
1	C	14	SER
1	C	39	LEU

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Mol	Chain	Res	Type
1	C	51	LYS
1	C	54	ILE
1	C	75	THR
1	C	78	THR
1	C	95	GLN
1	C	114	ARG
1	C	151	ASN
1	C	152	VAL
1	C	160	GLU
1	C	199	THR
1	C	203	THR
2	D	30	ASN
2	D	42	ARG
2	D	139	SER
2	D	161	VAL
2	D	171	SER
2	D	197	SER
2	D	199	ARG
3	G	146	ILE
3	G	155	GLU
3	G	225	ILE
3	G	226	THR
3	G	230	ARG
3	G	242	ASP
3	G	311	GLN
1	A	5	THR
1	A	13	VAL
1	A	14	SER
1	A	19	VAL
1	A	26	SER
1	A	27	GLN
1	A	39	LEU
1	A	51	LYS
1	A	54	ILE
1	A	75	THR
1	A	78	THR
1	A	84	VAL
1	A	95	GLN
1	A	114	ARG
1	A	142	LEU
1	A	151	ASN
1	A	152	VAL

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Mol	Chain	Res	Type
1	A	160	GLU
1	A	166	LEU
1	A	199	THR
1	A	203	THR
2	B	13	LEU
2	B	30	ASN
2	B	42	ARG
2	B	161	VAL
2	B	171	SER
2	B	184	ASP
2	B	197	SER
2	B	199	ARG
2	B	224	ARG
3	E	146	ILE
3	E	155	GLU
3	E	158	SER
3	E	172	SER
3	E	225	ILE
3	E	226	THR
3	E	230	ARG
3	E	242	ASP
3	E	278	GLU
3	E	290	LYS
3	E	309	GLN
3	E	311	GLN
3	E	319	ILE
3	E	320	GLU
1	F	5	THR
1	F	13	VAL
1	F	14	SER
1	F	19	VAL
1	F	27	GLN
1	F	39	LEU
1	F	54	ILE
1	F	75	THR
1	F	78	THR
1	F	84	VAL
1	F	95	GLN
1	F	114	ARG
1	F	151	ASN
1	F	152	VAL
1	F	160	GLU

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Mol	Chain	Res	Type
1	F	199	THR
1	F	203	THR
1	F	220	CYS
2	H	30	ASN
2	H	34	ILE
2	H	42	ARG
2	H	44	GLU
2	H	161	VAL
2	H	197	SER
2	H	199	ARG
3	I	146	ILE
3	I	155	GLU
3	I	158	SER
3	I	172	SER
3	I	225	ILE
3	I	226	THR
3	I	230	ARG
3	I	242	ASP
3	I	271	VAL
3	I	279	LYS
3	I	300	ASN
3	I	311	GLN
1	J	3	GLU
1	J	5	THR
1	J	13	VAL
1	J	14	SER
1	J	19	VAL
1	J	26	SER
1	J	27	GLN
1	J	39	LEU
1	J	46	PRO
1	J	51	LYS
1	J	54	ILE
1	J	75	THR
1	J	78	THR
1	J	84	VAL
1	J	95	GLN
1	J	114	ARG
1	J	142	LEU
1	J	151	ASN
1	J	152	VAL
1	J	160	GLU

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Mol	Chain	Res	Type
1	J	196	ASN
1	J	199	THR
1	J	203	THR
2	K	30	ASN
2	K	45	GLN
2	K	143	THR
2	K	161	VAL
2	K	197	SER
2	K	199	ARG
2	K	226	CYS
3	L	146	ILE
3	L	155	GLU
3	L	199	VAL
3	L	225	ILE
3	L	226	THR
3	L	230	ARG
3	L	242	ASP
3	L	309	GLN
3	L	311	GLN
3	L	319	ILE
3	L	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	44	GLN
1	C	95	GLN
1	C	167	ASN
1	C	195	HIS
2	D	41	GLN
2	D	84	GLN
3	G	148	HIS
3	G	224	ASN
3	G	227	ASN
3	G	282	GLN
3	G	309	GLN
3	G	311	GLN
1	A	27	GLN
1	A	44	GLN
1	A	95	GLN
1	A	143	ASN
1	A	167	ASN

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	216	ASN
2	B	41	GLN
2	B	103	HIS
3	E	224	ASN
3	E	309	GLN
3	E	311	GLN
1	F	95	GLN
1	F	143	ASN
1	F	167	ASN
2	H	3	GLN
2	H	142	GLN
2	H	175	HIS
2	H	182	GLN
3	I	227	ASN
3	I	311	GLN
1	J	27	GLN
1	J	43	GLN
1	J	44	GLN
1	J	95	GLN
1	J	163	ASN
1	J	167	ASN
1	J	196	ASN
2	K	3	GLN
2	K	41	GLN
2	K	103	HIS
3	L	194	ASN
3	L	301	ASN
3	L	309	GLN
3	L	311	GLN

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](#)

Of 49 ligands modelled in this entry, 12 are monoatomic - leaving 37 for Mogul analysis.

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	$\# Z > 2$
4	EDO	G	620	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	D	614	-	3,3,3	0.41	0	2,2,2	0.56	0
4	EDO	C	609	-	3,3,3	0.55	0	2,2,2	0.17	0
4	EDO	B	607	-	3,3,3	0.59	0	2,2,2	0.11	0
5	GOL	B	704	-	5,5,5	0.80	0	5,5,5	0.45	0
5	GOL	D	708	-	5,5,5	1.21	0	5,5,5	0.77	0
9	PEG	H	1000	-	6,6,6	0.46	0	5,5,5	0.57	0
4	EDO	B	616	-	3,3,3	0.50	0	2,2,2	0.15	0
4	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.39	0
4	EDO	B	624	-	3,3,3	0.47	0	2,2,2	0.22	0
4	EDO	L	610	-	3,3,3	0.50	0	2,2,2	0.32	0
4	EDO	A	625	-	3,3,3	0.42	0	2,2,2	0.35	0
5	GOL	D	702	-	5,5,5	0.77	0	5,5,5	1.03	1 (20%)
5	GOL	K	707	-	5,5,5	0.62	0	5,5,5	0.85	0
5	GOL	D	705	-	5,5,5	1.08	0	5,5,5	0.69	0
4	EDO	K	612	-	3,3,3	0.57	0	2,2,2	0.27	0
4	EDO	D	604	-	3,3,3	0.62	0	2,2,2	0.07	0
4	EDO	F	621	-	3,3,3	0.55	0	2,2,2	0.24	0
4	EDO	E	627	-	3,3,3	0.47	0	2,2,2	0.34	0
5	GOL	J	709	-	5,5,5	1.08	0	5,5,5	0.97	0
5	GOL	G	703	-	5,5,5	1.02	0	5,5,5	1.21	0
5	GOL	B	701	-	5,5,5	0.66	0	5,5,5	0.63	0
4	EDO	L	615	-	3,3,3	0.43	0	2,2,2	0.41	0
5	GOL	K	706	-	5,5,5	0.77	0	5,5,5	0.86	0
4	EDO	K	601	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	K	608	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	D	619	-	3,3,3	0.47	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	E	600	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	C	628	-	3,3,3	0.46	0	2,2,2	0.51	0
4	EDO	D	605	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	J	603	-	3,3,3	0.62	0	2,2,2	0.10	0
4	EDO	J	622	-	3,3,3	0.54	0	2,2,2	0.13	0
5	GOL	C	710	-	5,5,5	1.35	1 (20%)	5,5,5	1.42	1 (20%)
5	GOL	A	700	-	5,5,5	0.80	0	5,5,5	0.80	0
4	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	K	611	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	D	613	-	3,3,3	0.52	0	2,2,2	0.18	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
4	EDO	G	620	-	-	1/1/1/1	-
4	EDO	D	614	-	-	0/1/1/1	-
4	EDO	C	609	-	-	1/1/1/1	-
4	EDO	B	607	-	-	1/1/1/1	-
5	GOL	B	704	-	-	0/4/4/4	-
5	GOL	D	708	-	-	2/4/4/4	-
9	PEG	H	1000	-	-	2/4/4/4	-
4	EDO	B	616	-	-	1/1/1/1	-
4	EDO	A	618	-	-	0/1/1/1	-
4	EDO	B	624	-	-	0/1/1/1	-
4	EDO	L	610	-	-	0/1/1/1	-
4	EDO	A	625	-	-	0/1/1/1	-
5	GOL	D	702	-	-	2/4/4/4	-
5	GOL	K	707	-	-	2/4/4/4	-
5	GOL	D	705	-	-	4/4/4/4	-
4	EDO	K	612	-	-	0/1/1/1	-
4	EDO	D	604	-	-	1/1/1/1	-
4	EDO	F	621	-	-	1/1/1/1	-
4	EDO	E	627	-	-	0/1/1/1	-
5	GOL	J	709	-	-	2/4/4/4	-
5	GOL	G	703	-	-	3/4/4/4	-
5	GOL	B	701	-	-	0/4/4/4	-
4	EDO	L	615	-	-	1/1/1/1	-
5	GOL	K	706	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	K	601	-	-	1/1/1/1	-
4	EDO	K	608	-	-	0/1/1/1	-
4	EDO	D	619	-	-	1/1/1/1	-
4	EDO	E	600	-	-	0/1/1/1	-
4	EDO	C	628	-	-	0/1/1/1	-
4	EDO	D	605	-	-	1/1/1/1	-
4	EDO	J	603	-	-	1/1/1/1	-
4	EDO	J	622	-	-	0/1/1/1	-
5	GOL	C	710	-	-	0/4/4/4	-
5	GOL	A	700	-	-	0/4/4/4	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	K	611	-	-	1/1/1/1	-
4	EDO	D	613	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	710	GOL	O2-C2	2.03	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	710	GOL	O2-C2-C3	2.78	120.69	109.18
5	D	702	GOL	O1-C1-C2	2.20	120.30	110.38

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	702	GOL	O1-C1-C2-C3
5	D	705	GOL	O1-C1-C2-C3
5	D	705	GOL	C1-C2-C3-O3
5	D	708	GOL	O1-C1-C2-C3
5	J	709	GOL	O1-C1-C2-C3
5	K	706	GOL	O1-C1-C2-C3
5	K	707	GOL	O1-C1-C2-C3
5	K	707	GOL	O1-C1-C2-O2
5	G	703	GOL	O1-C1-C2-C3
5	G	703	GOL	C1-C2-C3-O3
5	D	702	GOL	O1-C1-C2-O2
5	D	705	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	708	GOL	O1-C1-C2-O2
5	J	709	GOL	O1-C1-C2-O2
4	F	621	EDO	O1-C1-C2-O2
4	J	603	EDO	O1-C1-C2-O2
9	H	1000	PEG	O1-C1-C2-O2
5	D	705	GOL	O1-C1-C2-O2
5	G	703	GOL	O1-C1-C2-O2
4	G	620	EDO	O1-C1-C2-O2
4	K	601	EDO	O1-C1-C2-O2
4	K	611	EDO	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2
4	D	619	EDO	O1-C1-C2-O2
5	K	706	GOL	O2-C2-C3-O3
9	H	1000	PEG	C4-C3-O2-C2
4	L	615	EDO	O1-C1-C2-O2
4	B	616	EDO	O1-C1-C2-O2
4	C	609	EDO	O1-C1-C2-O2
4	D	605	EDO	O1-C1-C2-O2
4	D	604	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	614	EDO	1	0
4	B	607	EDO	3	0
5	B	704	GOL	1	0
5	D	702	GOL	1	0
5	K	707	GOL	1	0
4	D	604	EDO	2	0
5	G	703	GOL	1	0
4	E	600	EDO	1	0
5	A	700	GOL	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	220/220 (100%)	0.09	2 (0%) 81 80	25, 42, 66, 94	0
1	C	220/220 (100%)	0.17	7 (3%) 50 46	26, 41, 80, 113	0
1	F	220/220 (100%)	1.37	45 (20%) 2 2	38, 74, 97, 112	0
1	J	220/220 (100%)	0.21	2 (0%) 81 80	26, 46, 66, 110	0
2	B	224/224 (100%)	0.01	5 (2%) 62 59	24, 39, 73, 105	0
2	D	224/224 (100%)	-0.08	4 (1%) 67 65	21, 37, 70, 113	0
2	H	224/224 (100%)	0.21	5 (2%) 62 59	28, 47, 77, 111	0
2	K	224/224 (100%)	0.20	5 (2%) 62 59	24, 41, 74, 111	0
3	E	189/190 (99%)	0.21	3 (1%) 70 68	28, 53, 76, 115	0
3	G	189/190 (99%)	0.04	3 (1%) 70 68	29, 44, 73, 104	0
3	I	189/190 (99%)	1.61	61 (32%) 1 1	42, 87, 116, 125	0
3	L	189/190 (99%)	1.30	44 (23%) 2 2	30, 73, 112, 122	0
All	All	2532/2536 (99%)	0.43	186 (7%) 21 18	21, 48, 98, 125	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	4	VAL	4.8
3	L	297	PHE	4.2
1	F	86	ALA	4.0
3	L	307	THR	4.0
3	I	319	ILE	3.9
3	L	308	ILE	3.9
1	F	211	ILE	3.9
3	I	292	PRO	3.7
3	E	319	ILE	3.7
3	I	237	LEU	3.7
3	I	234	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	4	VAL	3.6
3	I	296	VAL	3.5
1	F	200	CYS	3.5
1	A	163	ASN	3.5
1	F	154	TRP	3.5
3	I	172	SER	3.4
1	A	220	CYS	3.4
3	I	256	ILE	3.4
3	I	259	ALA	3.4
3	I	222	LEU	3.4
3	I	225	ILE	3.4
1	F	212	VAL	3.4
3	L	296	VAL	3.4
3	I	252	TYR	3.3
2	D	3	GLN	3.3
3	L	319	ILE	3.2
3	I	287	ILE	3.2
3	L	298	GLN	3.1
3	L	167	SER	3.1
3	L	168	LYS	3.1
1	F	8	PRO	3.1
3	I	311	GLN	3.1
2	B	4	VAL	3.1
3	L	132	ASP	3.0
1	F	206	THR	3.0
3	I	171	PHE	3.0
3	L	137	PHE	3.0
1	F	185	LEU	3.0
1	C	208	THR	2.9
3	L	267	TYR	2.9
3	I	218	VAL	2.9
1	F	156	ILE	2.8
3	I	269	ILE	2.8
3	I	134	ASP	2.8
2	K	226	CYS	2.8
1	F	147	PRO	2.8
1	C	164	GLY	2.8
3	I	226	THR	2.8
3	I	275	PHE	2.8
2	B	3	GLN	2.8
3	I	318	ALA	2.8
3	L	268	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	151	ARG	2.8
3	L	280	SER	2.8
3	I	238	VAL	2.7
3	I	293	ARG	2.7
3	I	317	PHE	2.7
1	F	187	LEU	2.7
3	I	185	THR	2.7
3	I	257	PRO	2.7
2	K	182	GLN	2.7
3	L	236	ILE	2.7
3	I	167	SER	2.7
3	L	194	ASN	2.7
3	L	300	ASN	2.7
1	F	80	THR	2.7
1	F	146	TYR	2.7
1	C	187	LEU	2.7
3	I	255	VAL	2.7
2	H	43	PRO	2.7
3	L	305	LEU	2.6
3	I	290	LYS	2.6
3	I	267	TYR	2.6
3	I	223	PHE	2.6
3	I	288	ALA	2.6
3	L	290	LYS	2.6
1	F	161	ARG	2.6
1	F	19	VAL	2.6
3	I	227	ASN	2.6
3	E	167	SER	2.5
3	L	287	ILE	2.5
3	L	281	ARG	2.5
3	L	315	LYS	2.5
1	F	152	VAL	2.5
3	I	136	ALA	2.5
1	C	159	SER	2.5
1	F	166	LEU	2.5
3	I	219	VAL	2.5
3	I	236	ILE	2.5
3	I	249	PRO	2.5
3	I	235	LYS	2.4
3	G	276	ARG	2.4
1	J	3	GLU	2.4
3	I	298	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	317	PHE	2.4
1	F	110	LEU	2.4
1	F	15	VAL	2.4
2	K	3	GLN	2.4
3	L	160	VAL	2.4
1	F	208	THR	2.4
1	F	109	LYS	2.4
1	F	153	LYS	2.4
3	I	251	GLY	2.4
1	F	38	TYR	2.4
2	H	181	LEU	2.4
2	B	143	THR	2.4
3	G	319	ILE	2.4
3	I	250	LEU	2.4
3	I	286	THR	2.4
3	L	292	PRO	2.4
1	F	121	VAL	2.4
2	D	181	LEU	2.3
2	B	181	LEU	2.3
3	L	312	LEU	2.3
3	I	316	ILE	2.3
3	L	306	LYS	2.3
3	I	291	PRO	2.3
1	F	84	VAL	2.3
3	L	271	VAL	2.3
3	I	135	ILE	2.3
1	F	148	LYS	2.3
1	F	10	SER	2.3
1	F	162	GLN	2.3
1	F	210	PRO	2.3
1	F	164	GLY	2.3
3	I	268	VAL	2.3
3	L	316	ILE	2.3
1	J	35	GLN	2.3
1	F	112	LEU	2.3
3	I	312	LEU	2.3
1	C	220	CYS	2.2
2	H	15	LYS	2.2
3	L	309	GLN	2.2
3	L	164	LEU	2.2
1	F	115	ALA	2.2
3	L	291	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	16	GLY	2.2
1	F	88	ASP	2.2
1	F	213	LYS	2.2
3	I	299	VAL	2.2
3	L	279	LYS	2.2
1	F	77	PHE	2.2
3	L	276	ARG	2.2
3	L	227	ASN	2.2
3	L	133	SER	2.2
3	I	276	ARG	2.2
1	F	81	ILE	2.2
3	L	218	VAL	2.2
3	G	320	GLU	2.1
1	F	194	ARG	2.1
1	F	85	LYS	2.1
3	I	168	LYS	2.1
1	F	2	ILE	2.1
3	I	294	ASP	2.1
3	I	289	SER	2.1
3	L	192	ASN	2.1
3	I	263	GLY	2.1
3	L	148	HIS	2.1
3	I	239	VAL	2.1
3	I	280	SER	2.1
3	L	314	GLU	2.1
3	E	166	LYS	2.1
1	F	119	PRO	2.1
2	H	3	GLN	2.1
2	K	144	ASN	2.1
1	C	211	ILE	2.1
1	F	18	LYS	2.1
2	D	45	GLN	2.1
3	L	190	GLN	2.1
2	D	226	CYS	2.1
3	I	184	PHE	2.1
3	I	246	PHE	2.1
3	I	297	PHE	2.1
3	L	302	PHE	2.1
1	C	160	GLU	2.0
1	F	117	ALA	2.0
3	I	233	ALA	2.0
3	L	278	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	I	148	HIS	2.0
3	L	225	ILE	2.0
3	I	261	ARG	2.0
1	F	202	ALA	2.0
3	I	277	SER	2.0
1	F	108	THR	2.0
2	B	142	GLN	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	B	616	4/4	0.65	0.25	63,64,64,65	0
4	EDO	D	614	4/4	0.69	0.18	49,49,50,51	0
4	EDO	A	618	4/4	0.71	0.18	57,59,62,62	0
5	GOL	C	710	6/6	0.74	0.17	53,56,57,58	0
5	GOL	D	702	6/6	0.74	0.19	61,63,64,64	0
4	EDO	K	608	4/4	0.75	0.14	52,56,56,60	0
4	EDO	L	610	4/4	0.75	0.16	57,58,58,65	0
4	EDO	K	611	4/4	0.77	0.18	60,62,62,65	0
5	GOL	D	705	6/6	0.77	0.17	59,61,61,62	0
5	GOL	A	700	6/6	0.78	0.17	68,69,70,71	0
5	GOL	B	701	6/6	0.78	0.14	71,71,72,73	0
8	CL	J	903	1/1	0.78	0.21	70,70,70,70	0
5	GOL	D	708	6/6	0.79	0.15	50,50,51,51	0
4	EDO	J	622	4/4	0.79	0.18	55,56,57,66	0
4	EDO	F	621	4/4	0.80	0.18	56,57,58,62	0
5	GOL	K	707	6/6	0.80	0.15	66,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	619	4/4	0.80	0.21	53,55,57,60	0
9	PEG	H	1000	7/7	0.80	0.16	59,59,62,63	0
5	GOL	K	706	6/6	0.81	0.15	60,62,62,62	0
4	EDO	L	615	4/4	0.81	0.11	51,54,55,55	0
6	NA	H	801	1/1	0.82	0.17	37,37,37,37	0
4	EDO	C	609	4/4	0.82	0.18	54,54,56,57	0
5	GOL	J	709	6/6	0.82	0.14	59,60,61,62	0
4	EDO	B	607	4/4	0.83	0.17	47,50,51,55	0
4	EDO	K	612	4/4	0.83	0.12	39,40,41,42	0
4	EDO	D	605	4/4	0.84	0.16	49,50,50,55	0
5	GOL	B	704	6/6	0.84	0.19	54,56,56,57	0
4	EDO	A	625	4/4	0.85	0.13	41,43,45,45	0
4	EDO	D	604	4/4	0.86	0.14	37,40,41,48	0
4	EDO	B	624	4/4	0.86	0.14	55,55,56,64	0
8	CL	G	907	1/1	0.86	0.11	74,74,74,74	0
4	EDO	E	600	4/4	0.86	0.17	42,43,48,49	0
4	EDO	E	627	4/4	0.86	0.14	54,57,60,62	0
4	EDO	B	606	4/4	0.87	0.11	43,43,47,48	0
5	GOL	G	703	6/6	0.87	0.11	48,48,49,49	0
4	EDO	C	628	4/4	0.87	0.13	50,50,52,56	0
4	EDO	J	603	4/4	0.88	0.12	40,42,45,45	0
4	EDO	D	613	4/4	0.88	0.13	51,51,55,58	0
8	CL	E	902	1/1	0.91	0.06	60,60,60,60	0
4	EDO	G	620	4/4	0.91	0.11	38,38,39,46	0
8	CL	K	904	1/1	0.91	0.08	63,63,63,63	0
4	EDO	K	601	4/4	0.91	0.11	40,40,41,46	0
6	NA	D	800	1/1	0.92	0.17	41,41,41,41	0
6	NA	H	802	1/1	0.93	0.27	58,58,58,58	0
8	CL	E	906	1/1	0.97	0.07	71,71,71,71	0
7	CA	L	500	1/1	0.97	0.04	40,40,40,40	0
7	CA	E	500	1/1	0.97	0.03	40,40,40,40	0
7	CA	I	500	1/1	0.97	0.04	57,57,57,57	0
7	CA	G	500	1/1	0.99	0.03	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.