



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 11:36 AM EST

PDB ID : 3Q3G
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

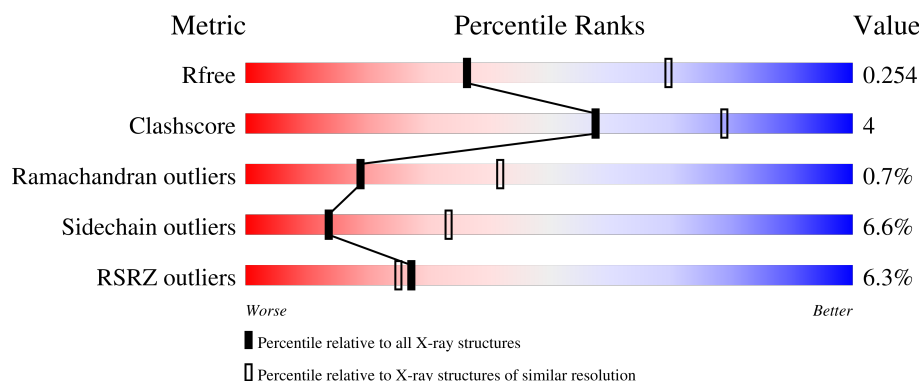
1 Overall quality at a glance

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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	<div> <div>0%</div> <div> <div>82%</div> <div>16%</div> <div>•</div> </div> </div>
1	C	220	<div> <div>2%</div> <div> <div>84%</div> <div>15%</div> <div>•</div> </div> </div>
1	F	220	<div> <div>18%</div> <div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>
1	J	220	<div> <div>0%</div> <div> <div>81%</div> <div>16%</div> <div>•</div> </div> </div>
2	B	224	<div> <div>2%</div> <div> <div>85%</div> <div>13%</div> <div>•</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	224	<div><div></div><div>%</div><div>83%</div><div>15%</div><div>•</div></div>
2	H	224	<div><div></div><div>2%</div><div>84%</div><div>15%</div><div>•</div></div>
2	K	224	<div><div></div><div>2%</div><div>87%</div><div>13%</div><div></div></div>
3	E	190	<div><div></div><div>%</div><div>87%</div><div>11%</div><div>••</div></div>
3	G	190	<div><div></div><div>2%</div><div>84%</div><div>15%</div><div>••</div></div>
3	I	190	<div><div></div><div>27%</div><div>85%</div><div>14%</div><div>••</div></div>
3	L	190	<div><div></div><div>21%</div><div>83%</div><div>14%</div><div>••</div></div>

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 (three-letter code: EDO) (formula: C₂H₆O₂).



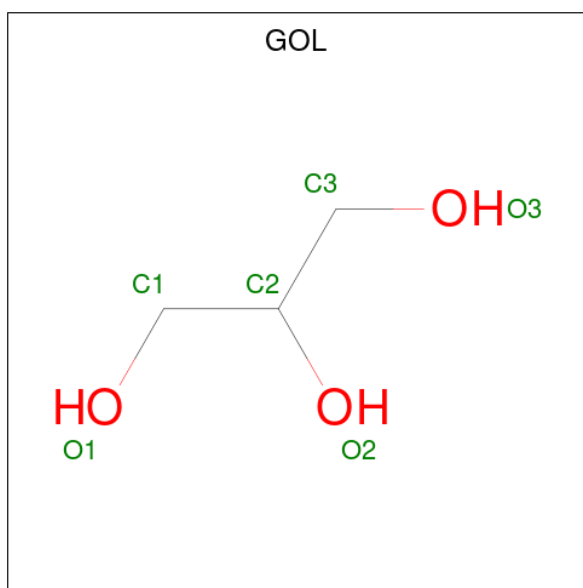
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

Continued on next page...

Continued from previous page...

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 (three-letter code: 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 (three-letter code: 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

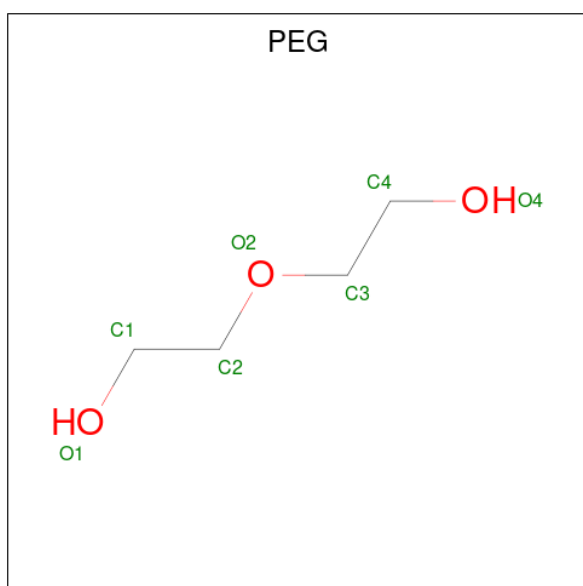
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-letter code: 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 (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

Continued on next page...

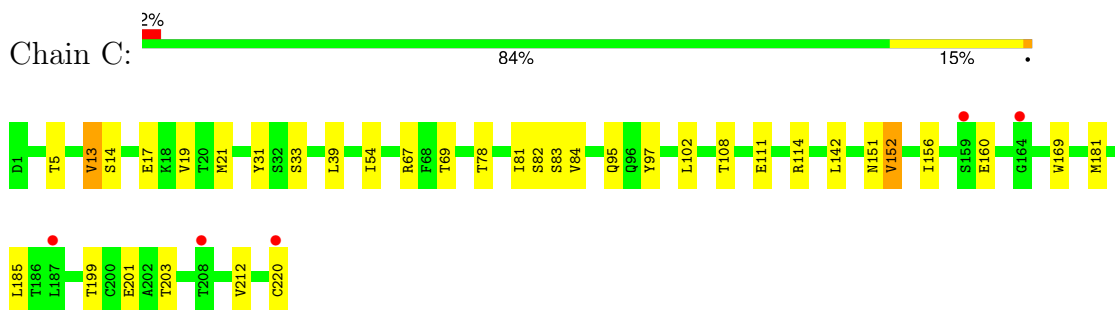
Continued from previous page...

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

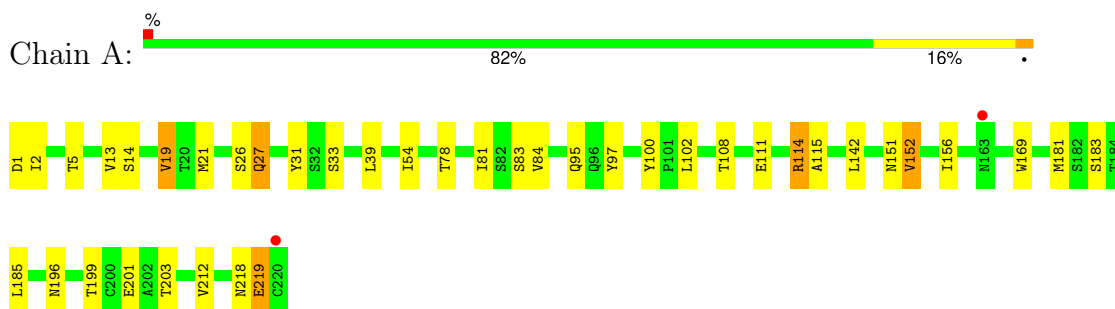
3 Residue-property plots [i](#)

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.

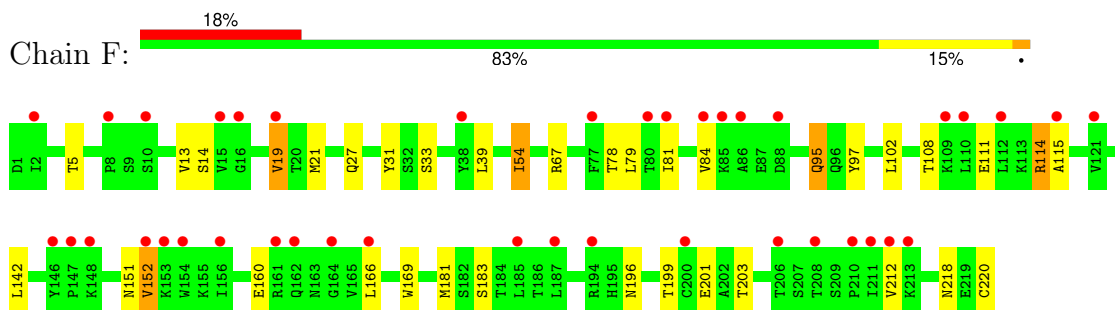
• Molecule 1: Antibody Light Chain



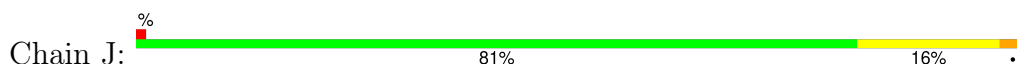
• Molecule 1: Antibody Light Chain

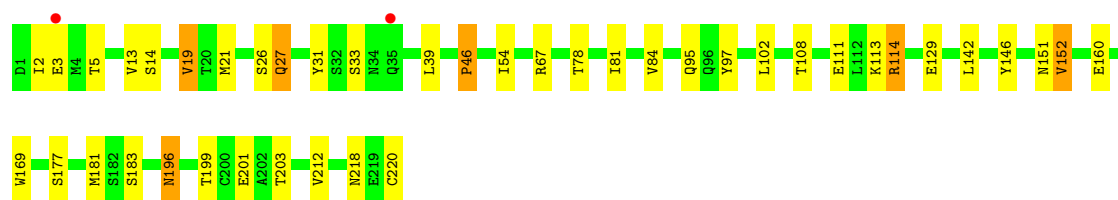


• Molecule 1: Antibody Light Chain

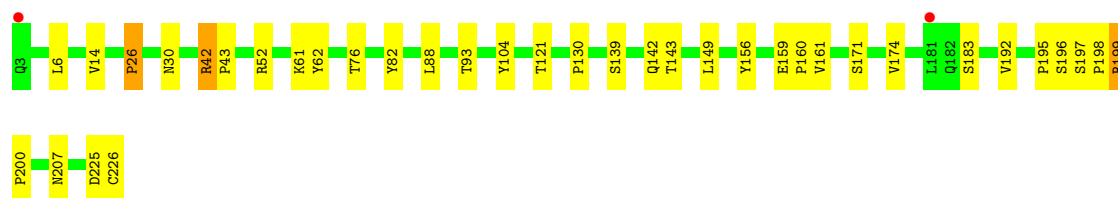
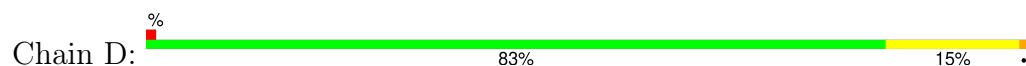


• Molecule 1: Antibody Light Chain

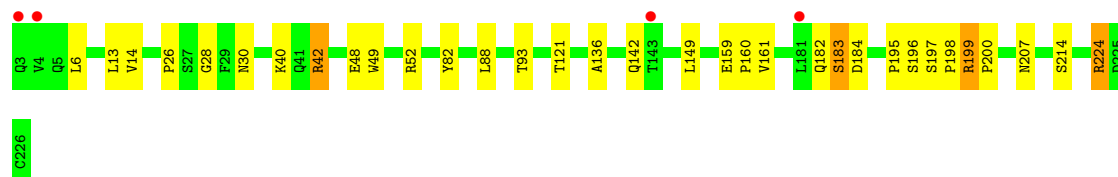
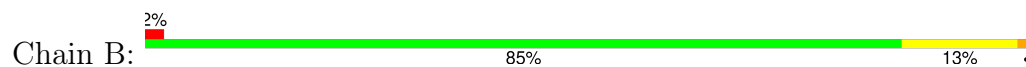




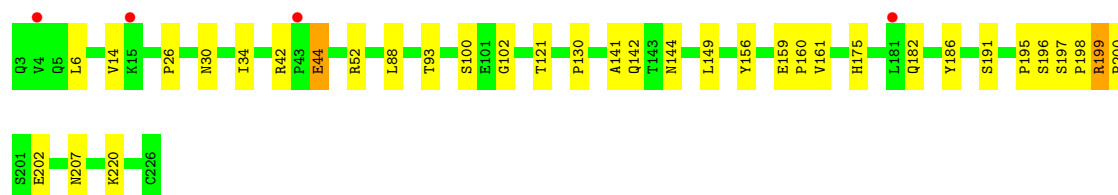
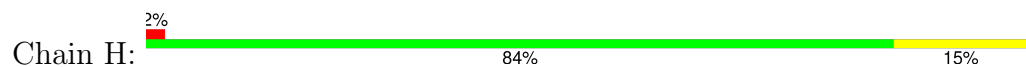
• Molecule 2: Antibody Heavy chain



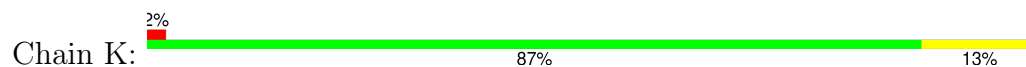
• Molecule 2: Antibody Heavy chain



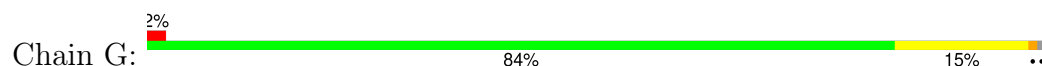
• Molecule 2: Antibody Heavy chain

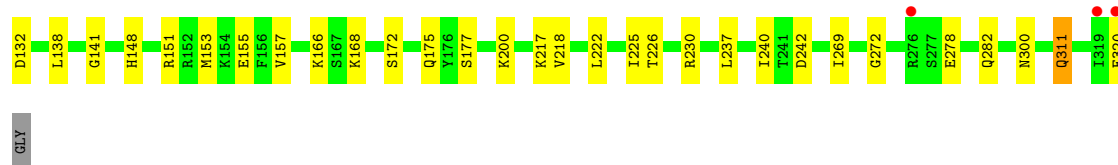


• Molecule 2: Antibody Heavy chain

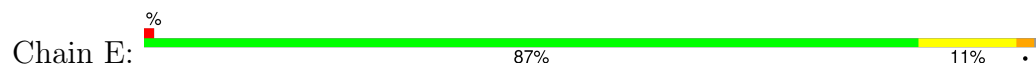


• Molecule 3: Integrin alpha-M

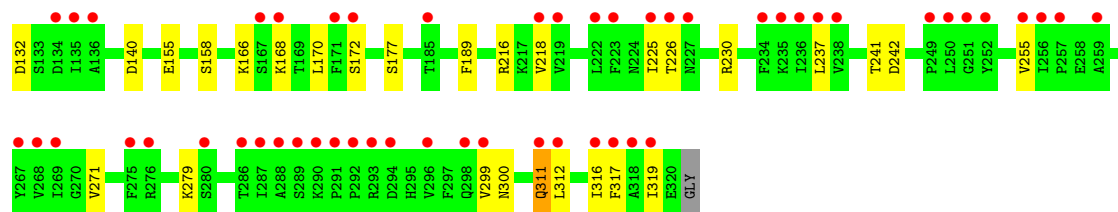
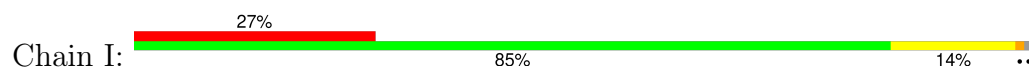




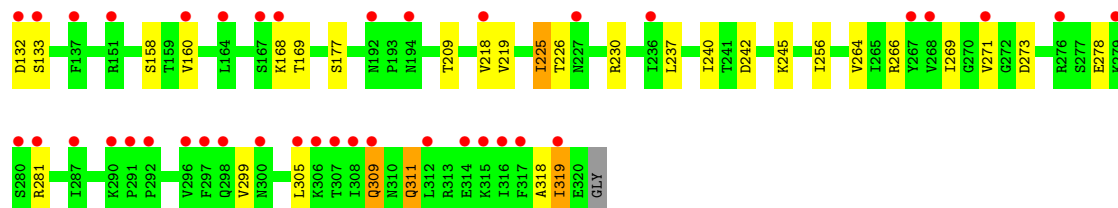
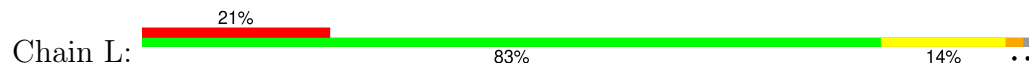
• Molecule 3: Integrin alpha-M



• 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	4048 reflections (5.00%)	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, GOL, NA, CL, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1757	0.71	1/2384 (0.0%)
1	C	0.44	0/1757	0.69	0/2384
1	F	0.40	0/1757	0.68	0/2384
1	J	0.44	0/1757	0.74	0/2384
2	B	0.44	0/1732	0.74	0/2368
2	D	0.45	0/1732	0.75	0/2368
2	H	0.44	0/1732	0.74	0/2368
2	K	0.45	0/1732	0.74	0/2368
3	E	0.44	0/1560	0.71	1/2099 (0.0%)
3	G	0.46	0/1560	0.70	0/2099
3	I	0.45	0/1560	0.67	0/2099
3	L	0.47	0/1560	0.70	0/2099
All	All	0.44	0/20196	0.71	2/27404 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	GLU	C-N-CA	5.51	135.47	121.70
3	E	167	SER	N-CA-C	-5.27	96.76	111.00

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	1718	0	1647	14	0
1	C	1718	0	1647	14	0
1	F	1718	0	1647	14	0
1	J	1718	0	1647	14	0
2	B	1689	0	1638	21	0
2	D	1689	0	1638	21	0
2	H	1689	0	1638	20	0
2	K	1689	0	1638	18	0
3	E	1531	0	1545	6	0
3	G	1531	0	1545	14	0
3	I	1531	0	1545	10	0
3	L	1531	0	1545	16	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	49	0	0	0	0
10	C	42	0	0	1	0
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	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (174) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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

Continued on next page...

Continued from previous page...

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
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:181:MET:HE3	1:F:183:SER:HB2	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
1:J:129:GLU:HG2	2:K:219:LYS:HZ1	1.84	0.42
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:J:181:MET:HE3	1:J:183:SER:HB2	2.02	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
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
1:A:181:MET:HE3	1:A:183:SER:HB2	2.04	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%)	25	49
1	F	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
1	J	218/220 (99%)	211 (97%)	6 (3%)	1 (0%)	25	49
2	B	222/224 (99%)	210 (95%)	10 (4%)	2 (1%)	14	35
2	D	222/224 (99%)	212 (96%)	6 (3%)	4 (2%)	7	18
2	H	222/224 (99%)	211 (95%)	10 (4%)	1 (0%)	25	49
2	K	222/224 (99%)	213 (96%)	8 (4%)	1 (0%)	25	49
3	E	187/190 (98%)	178 (95%)	7 (4%)	2 (1%)	12	30
3	G	187/190 (98%)	179 (96%)	7 (4%)	1 (0%)	25	49
3	I	187/190 (98%)	180 (96%)	5 (3%)	2 (1%)	12	30
3	L	187/190 (98%)	178 (95%)	8 (4%)	1 (0%)	25	49
All	All	2508/2536 (99%)	2407 (96%)	83 (3%)	18 (1%)	19	42

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
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%)	180 (91%)	17 (9%)	8	21
1	C	197/197 (100%)	183 (93%)	14 (7%)	12	30
1	F	197/197 (100%)	179 (91%)	18 (9%)	7	19
1	J	197/197 (100%)	175 (89%)	22 (11%)	5	12
2	B	192/192 (100%)	181 (94%)	11 (6%)	17	40
2	D	192/192 (100%)	181 (94%)	11 (6%)	17	40
2	H	192/192 (100%)	184 (96%)	8 (4%)	25	53
2	K	192/192 (100%)	183 (95%)	9 (5%)	22	49
3	E	169/169 (100%)	156 (92%)	13 (8%)	10	26
3	G	169/169 (100%)	163 (96%)	6 (4%)	30	59
3	I	169/169 (100%)	159 (94%)	10 (6%)	16	38
3	L	169/169 (100%)	160 (95%)	9 (5%)	19	43
All	All	2232/2232 (100%)	2084 (93%)	148 (7%)	14	33

All (148) 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
1	C	54	ILE
1	C	78	THR
1	C	95	GLN
1	C	111	GLU
1	C	114	ARG
1	C	151	ASN
1	C	152	VAL
1	C	160	GLU
1	C	199	THR
1	C	203	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	26	PRO
2	D	30	ASN
2	D	42	ARG
2	D	52	ARG
2	D	139	SER
2	D	161	VAL
2	D	171	SER
2	D	196	SER
2	D	197	SER
2	D	199	ARG
2	D	207	ASN
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	54	ILE
1	A	78	THR
1	A	84	VAL
1	A	95	GLN
1	A	111	GLU
1	A	114	ARG
1	A	151	ASN
1	A	152	VAL
1	A	199	THR
1	A	203	THR
2	B	13	LEU
2	B	30	ASN
2	B	42	ARG
2	B	52	ARG
2	B	161	VAL
2	B	184	ASP
2	B	196	SER
2	B	197	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	199	ARG
2	B	207	ASN
2	B	224	ARG
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	245	LYS
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	78	THR
1	F	84	VAL
1	F	95	GLN
1	F	111	GLU
1	F	114	ARG
1	F	151	ASN
1	F	152	VAL
1	F	160	GLU
1	F	199	THR
1	F	203	THR
1	F	220	CYS
2	H	30	ASN
2	H	44	GLU
2	H	52	ARG
2	H	161	VAL
2	H	196	SER
2	H	197	SER
2	H	199	ARG
2	H	207	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	54	ILE
1	J	78	THR
1	J	84	VAL
1	J	95	GLN
1	J	111	GLU
1	J	114	ARG
1	J	151	ASN
1	J	152	VAL
1	J	160	GLU
1	J	196	ASN
1	J	199	THR
1	J	203	THR
1	J	220	CYS
2	K	30	ASN
2	K	52	ARG
2	K	143	THR
2	K	161	VAL
2	K	184	ASP
2	K	196	SER
2	K	197	SER
2	K	199	ARG
2	K	226	CYS
3	L	158	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	225	ILE
3	L	226	THR
3	L	230	ARG
3	L	242	ASP
3	L	273	ASP
3	L	309	GLN
3	L	311	GLN
3	L	319	ILE

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	35	GLN
1	C	44	GLN
1	C	95	GLN
1	C	167	ASN
2	D	41	GLN
3	G	148	HIS
3	G	224	ASN
3	G	227	ASN
3	G	282	GLN
3	G	311	GLN
1	A	27	GLN
1	A	35	GLN
1	A	44	GLN
1	A	95	GLN
1	A	167	ASN
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	27	GLN
1	F	35	GLN
1	F	44	GLN
1	F	95	GLN
1	F	167	ASN
2	H	41	GLN
2	H	144	ASN
2	H	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	182	GLN
3	I	210	HIS
3	I	224	ASN
3	I	227	ASN
3	I	309	GLN
3	I	311	GLN
1	J	27	GLN
1	J	35	GLN
1	J	44	GLN
1	J	95	GLN
1	J	167	ASN
1	J	196	ASN
2	K	41	GLN
3	L	224	ASN
3	L	282	GLN
3	L	309	GLN
3	L	311	GLN

5.3.3 RNA [i](#)

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](#)

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	K	611	-	3,3,3	0.52	0	2,2,2	0.22	0
4	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.39	0
4	EDO	J	603	-	3,3,3	0.62	0	2,2,2	0.10	0
5	GOL	G	703	-	5,5,5	1.02	0	5,5,5	1.21	0
5	GOL	C	710	-	5,5,5	1.35	1 (20%)	5,5,5	1.42	1 (20%)
4	EDO	J	622	-	3,3,3	0.54	0	2,2,2	0.13	0
4	EDO	L	615	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	D	619	-	3,3,3	0.47	0	2,2,2	0.38	0
4	EDO	G	620	-	3,3,3	0.42	0	2,2,2	0.43	0
4	EDO	F	621	-	3,3,3	0.55	0	2,2,2	0.24	0
5	GOL	D	702	-	5,5,5	0.77	0	5,5,5	1.03	1 (20%)
4	EDO	D	604	-	3,3,3	0.62	0	2,2,2	0.07	0
5	GOL	J	709	-	5,5,5	1.08	0	5,5,5	0.97	0
4	EDO	B	607	-	3,3,3	0.59	0	2,2,2	0.11	0
4	EDO	D	613	-	3,3,3	0.52	0	2,2,2	0.18	0
4	EDO	K	608	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	E	600	-	3,3,3	0.48	0	2,2,2	0.29	0
5	GOL	B	704	-	5,5,5	0.80	0	5,5,5	0.45	0
4	EDO	D	614	-	3,3,3	0.41	0	2,2,2	0.56	0
5	GOL	K	706	-	5,5,5	0.77	0	5,5,5	0.86	0
5	GOL	D	705	-	5,5,5	1.08	0	5,5,5	0.69	0
5	GOL	K	707	-	5,5,5	0.62	0	5,5,5	0.85	0
5	GOL	B	701	-	5,5,5	0.66	0	5,5,5	0.63	0
4	EDO	B	616	-	3,3,3	0.50	0	2,2,2	0.15	0
9	PEG	H	1000	-	6,6,6	0.46	0	5,5,5	0.57	0
4	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	C	609	-	3,3,3	0.55	0	2,2,2	0.17	0
4	EDO	A	625	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	K	612	-	3,3,3	0.57	0	2,2,2	0.27	0
4	EDO	D	605	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	L	610	-	3,3,3	0.50	0	2,2,2	0.32	0
5	GOL	D	708	-	5,5,5	1.21	0	5,5,5	0.77	0
5	GOL	A	700	-	5,5,5	0.80	0	5,5,5	0.80	0
4	EDO	C	628	-	3,3,3	0.46	0	2,2,2	0.51	0
4	EDO	K	601	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	E	627	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	B	624	-	3,3,3	0.47	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
4	EDO	K	611	-	-	1/1/1/1	-
4	EDO	A	618	-	-	0/1/1/1	-
4	EDO	J	603	-	-	1/1/1/1	-
5	GOL	G	703	-	-	3/4/4/4	-
5	GOL	C	710	-	-	0/4/4/4	-
4	EDO	J	622	-	-	0/1/1/1	-
4	EDO	L	615	-	-	1/1/1/1	-
4	EDO	D	619	-	-	1/1/1/1	-
4	EDO	G	620	-	-	1/1/1/1	-
4	EDO	F	621	-	-	1/1/1/1	-
5	GOL	D	702	-	-	2/4/4/4	-
4	EDO	D	604	-	-	1/1/1/1	-
5	GOL	J	709	-	-	2/4/4/4	-
4	EDO	B	607	-	-	1/1/1/1	-
4	EDO	D	613	-	-	0/1/1/1	-
4	EDO	K	608	-	-	0/1/1/1	-
4	EDO	E	600	-	-	0/1/1/1	-
5	GOL	B	704	-	-	0/4/4/4	-
4	EDO	D	614	-	-	0/1/1/1	-
5	GOL	K	706	-	-	2/4/4/4	-
5	GOL	D	705	-	-	4/4/4/4	-
5	GOL	K	707	-	-	2/4/4/4	-
5	GOL	B	701	-	-	0/4/4/4	-
4	EDO	B	616	-	-	1/1/1/1	-
9	PEG	H	1000	-	-	2/4/4/4	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	C	609	-	-	1/1/1/1	-
4	EDO	A	625	-	-	0/1/1/1	-
4	EDO	K	612	-	-	0/1/1/1	-
4	EDO	D	605	-	-	1/1/1/1	-
4	EDO	L	610	-	-	0/1/1/1	-
5	GOL	D	708	-	-	2/4/4/4	-
5	GOL	A	700	-	-	0/4/4/4	-
4	EDO	C	628	-	-	0/1/1/1	-
4	EDO	K	601	-	-	1/1/1/1	-
4	EDO	E	627	-	-	0/1/1/1	-
4	EDO	B	624	-	-	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
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
5	G	703	GOL	1	0
5	D	702	GOL	1	0
4	D	604	EDO	2	0
4	B	607	EDO	3	0
4	E	600	EDO	1	0
5	B	704	GOL	1	0
4	D	614	EDO	1	0
5	K	707	GOL	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%)	-0.04	2 (0%) 81 80	25, 42, 66, 94	0
1	C	220/220 (100%)	0.04	5 (2%) 61 60	26, 41, 80, 113	0
1	F	220/220 (100%)	1.26	40 (18%) 4 4	38, 74, 97, 112	0
1	J	220/220 (100%)	0.07	2 (0%) 81 80	26, 46, 66, 110	0
2	B	224/224 (100%)	-0.12	4 (1%) 67 67	24, 39, 73, 105	0
2	D	224/224 (100%)	-0.21	2 (0%) 81 80	21, 37, 70, 113	0
2	H	224/224 (100%)	0.08	4 (1%) 67 67	28, 47, 77, 111	0
2	K	224/224 (100%)	0.07	4 (1%) 67 67	24, 41, 74, 111	0
3	E	189/190 (99%)	0.08	2 (1%) 77 77	28, 53, 76, 115	0
3	G	189/190 (99%)	-0.09	3 (1%) 70 70	29, 44, 73, 104	0
3	I	189/190 (99%)	1.49	52 (27%) 2 2	42, 87, 116, 125	0
3	L	189/190 (99%)	1.19	39 (20%) 3 3	30, 73, 112, 122	0
All	All	2532/2536 (99%)	0.30	159 (6%) 27 25	21, 48, 98, 125	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	4	VAL	4.7
3	L	297	PHE	4.0
1	F	86	ALA	3.9
3	L	307	THR	3.9
3	I	319	ILE	3.8
3	L	308	ILE	3.8
1	F	211	ILE	3.8
3	I	292	PRO	3.6
3	E	319	ILE	3.6
3	I	237	LEU	3.6
2	H	4	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	234	PHE	3.5
1	A	163	ASN	3.4
3	I	296	VAL	3.4
1	F	200	CYS	3.4
3	I	172	SER	3.4
1	F	154	TRP	3.3
1	A	220	CYS	3.3
3	I	256	ILE	3.3
3	I	259	ALA	3.3
3	I	225	ILE	3.3
3	I	222	LEU	3.3
1	F	212	VAL	3.2
3	L	296	VAL	3.2
3	I	252	TYR	3.2
2	D	3	GLN	3.2
3	L	319	ILE	3.1
3	I	287	ILE	3.1
3	L	298	GLN	3.0
3	L	167	SER	3.0
3	L	168	LYS	3.0
3	I	311	GLN	3.0
1	F	8	PRO	3.0
3	L	132	ASP	2.9
2	B	4	VAL	2.9
1	F	206	THR	2.9
1	F	185	LEU	2.9
1	C	208	THR	2.8
3	I	171	PHE	2.8
3	L	137	PHE	2.8
3	L	267	TYR	2.8
3	I	134	ASP	2.8
3	I	218	VAL	2.7
3	L	151	ARG	2.7
1	F	156	ILE	2.7
3	I	269	ILE	2.7
2	K	226	CYS	2.7
2	B	3	GLN	2.7
1	F	147	PRO	2.7
3	I	226	THR	2.7
3	L	280	SER	2.7
1	C	164	GLY	2.7
3	I	293	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	268	VAL	2.7
3	I	275	PHE	2.7
3	I	318	ALA	2.7
3	I	238	VAL	2.6
2	K	182	GLN	2.6
3	I	185	THR	2.6
3	I	167	SER	2.6
3	L	194	ASN	2.6
3	L	300	ASN	2.6
1	F	187	LEU	2.6
3	I	257	PRO	2.6
3	I	317	PHE	2.6
1	F	80	THR	2.6
3	L	236	ILE	2.6
3	I	290	LYS	2.5
1	F	146	TYR	2.5
1	C	187	LEU	2.5
2	H	43	PRO	2.5
3	I	255	VAL	2.5
3	L	305	LEU	2.5
1	F	161	ARG	2.5
3	L	290	LYS	2.5
3	I	267	TYR	2.5
3	L	281	ARG	2.5
3	I	288	ALA	2.5
3	E	167	SER	2.5
3	I	223	PHE	2.5
3	I	227	ASN	2.5
3	L	315	LYS	2.5
1	C	159	SER	2.4
1	F	19	VAL	2.4
3	L	287	ILE	2.4
1	F	152	VAL	2.4
3	I	136	ALA	2.4
1	F	166	LEU	2.4
3	G	276	ARG	2.4
3	I	219	VAL	2.4
3	I	236	ILE	2.4
1	J	3	GLU	2.4
3	I	235	LYS	2.4
3	I	249	PRO	2.4
3	I	298	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	3	GLN	2.3
1	F	110	LEU	2.3
1	F	109	LYS	2.3
1	F	153	LYS	2.3
1	F	208	THR	2.3
1	F	15	VAL	2.3
3	L	160	VAL	2.3
3	L	317	PHE	2.3
2	B	143	THR	2.3
3	I	286	THR	2.3
3	G	319	ILE	2.3
3	I	251	GLY	2.3
2	H	181	LEU	2.3
3	I	250	LEU	2.3
3	L	306	LYS	2.2
1	F	38	TYR	2.2
3	L	292	PRO	2.2
1	F	121	VAL	2.2
3	I	316	ILE	2.2
1	F	148	LYS	2.2
2	D	181	LEU	2.2
2	B	181	LEU	2.2
3	L	312	LEU	2.2
1	F	10	SER	2.2
3	I	291	PRO	2.2
1	F	84	VAL	2.2
1	F	162	GLN	2.2
3	L	271	VAL	2.2
3	I	135	ILE	2.2
1	F	210	PRO	2.2
1	J	35	GLN	2.2
3	I	268	VAL	2.2
3	L	316	ILE	2.2
2	H	15	LYS	2.2
1	F	164	GLY	2.2
3	L	309	GLN	2.1
1	F	112	LEU	2.1
3	I	312	LEU	2.1
1	C	220	CYS	2.1
3	L	276	ARG	2.1
1	F	213	LYS	2.1
3	L	279	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	88	ASP	2.1
3	L	164	LEU	2.1
1	F	115	ALA	2.1
3	I	276	ARG	2.1
3	L	291	PRO	2.1
3	L	133	SER	2.1
3	I	299	VAL	2.1
3	L	227	ASN	2.1
1	F	194	ARG	2.1
1	F	16	GLY	2.1
3	G	320	GLU	2.1
1	F	77	PHE	2.1
1	F	85	LYS	2.0
3	I	168	LYS	2.0
1	F	81	ILE	2.0
3	I	289	SER	2.0
3	L	218	VAL	2.0
3	I	294	ASP	2.0
3	L	314	GLU	2.0
1	F	2	ILE	2.0
3	I	280	SER	2.0
3	L	192	ASN	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 monosaccharides 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(\AA^2)	Q<0.9
4	EDO	B	616	4/4	0.65	0.25	63,64,64,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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 [i](#)

There are no such residues in this entry.