



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:03 PM UTC

PDB ID : 7STZ / pdb_00007stz
Title : Crystal Structure of Human E-cadherin EC1-5 bound by mouse monoclonal antibody Fab mAb-1_19A11
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-11-15
Resolution : 2.95 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

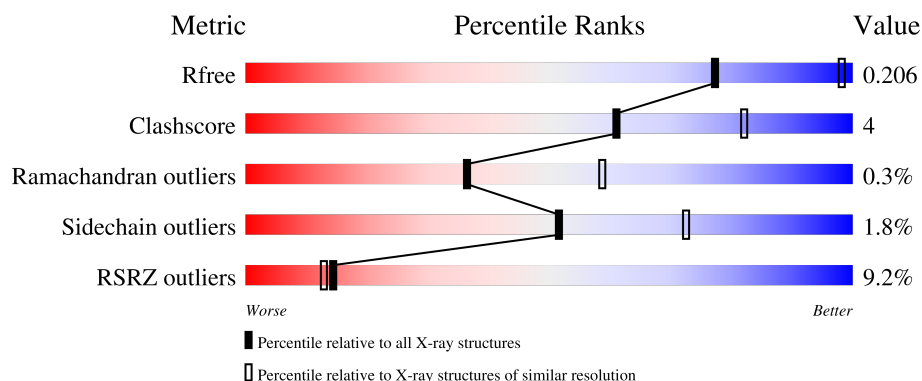
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	C	590	8% 77% 13% • 8%
1	D	590	16% 63% 9% 28%
2	H	246	6% 80% 9% 11%
2	I	246	3% 77% 10% 12%
3	L	240	0% 83% 9% 8%

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Mol	Chain	Length	Quality of chain
3	M	240	% 84% 8% 8%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14687 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 Cadherin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	540	Total	C	N	O	S	0	1	0
			4093	2572	660	851	10			
1	D	422	Total	C	N	O	S	0	0	0
			3068	1910	498	656	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	expression tag	UNP P12830
C	-14	PRO	-	expression tag	UNP P12830
C	-13	LEU	-	expression tag	UNP P12830
C	-12	LEU	-	expression tag	UNP P12830
C	-11	LEU	-	expression tag	UNP P12830
C	-10	LEU	-	expression tag	UNP P12830
C	-9	LEU	-	expression tag	UNP P12830
C	-8	PRO	-	expression tag	UNP P12830
C	-7	LEU	-	expression tag	UNP P12830
C	-6	LEU	-	expression tag	UNP P12830
C	-5	TRP	-	expression tag	UNP P12830
C	-4	ALA	-	expression tag	UNP P12830
C	-3	GLY	-	expression tag	UNP P12830
C	-2	ALA	-	expression tag	UNP P12830
C	-1	LEU	-	expression tag	UNP P12830
C	0	ALA	-	expression tag	UNP P12830
D	-15	MET	-	expression tag	UNP P12830
D	-14	PRO	-	expression tag	UNP P12830
D	-13	LEU	-	expression tag	UNP P12830
D	-12	LEU	-	expression tag	UNP P12830
D	-11	LEU	-	expression tag	UNP P12830
D	-10	LEU	-	expression tag	UNP P12830
D	-9	LEU	-	expression tag	UNP P12830
D	-8	PRO	-	expression tag	UNP P12830
D	-7	LEU	-	expression tag	UNP P12830

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	LEU	-	expression tag	UNP P12830
D	-5	TRP	-	expression tag	UNP P12830
D	-4	ALA	-	expression tag	UNP P12830
D	-3	GLY	-	expression tag	UNP P12830
D	-2	ALA	-	expression tag	UNP P12830
D	-1	LEU	-	expression tag	UNP P12830
D	0	ALA	-	expression tag	UNP P12830

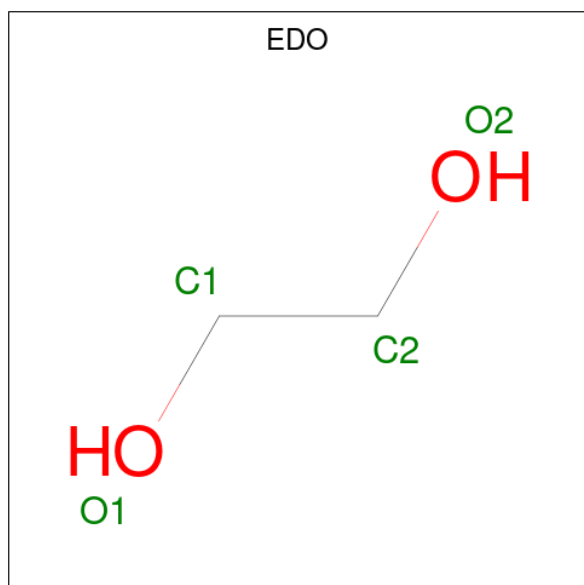
- Molecule 2 is a protein called mAb-1_19A11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	5	0
			1643	1042	268	322	11			
2	I	216	Total	C	N	O	S	0	6	0
			1646	1041	273	322	10			

- Molecule 3 is a protein called mAb-1_19A11 Light Chain.

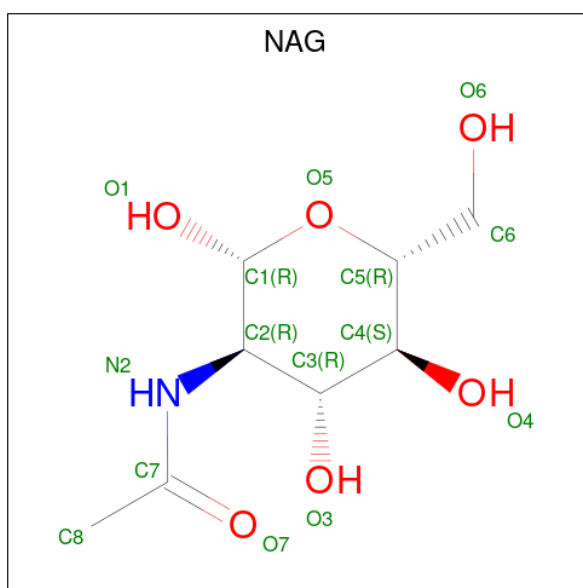
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	220	Total	C	N	O	S	0	2	0
			1703	1060	289	345	9			
3	M	220	Total	C	N	O	S	0	2	0
			1712	1066	293	345	8			

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



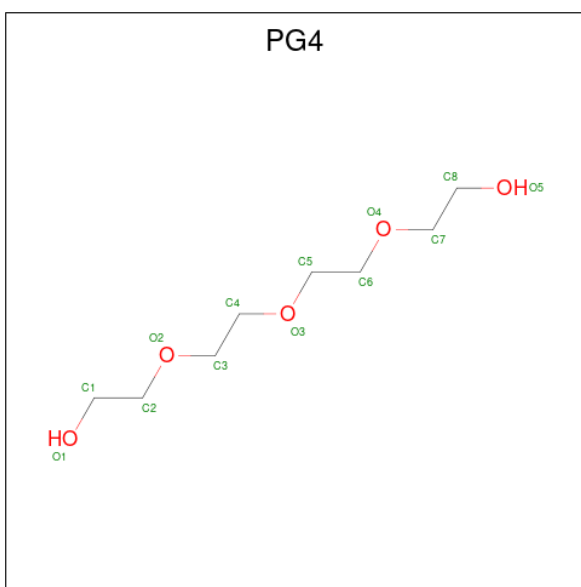
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



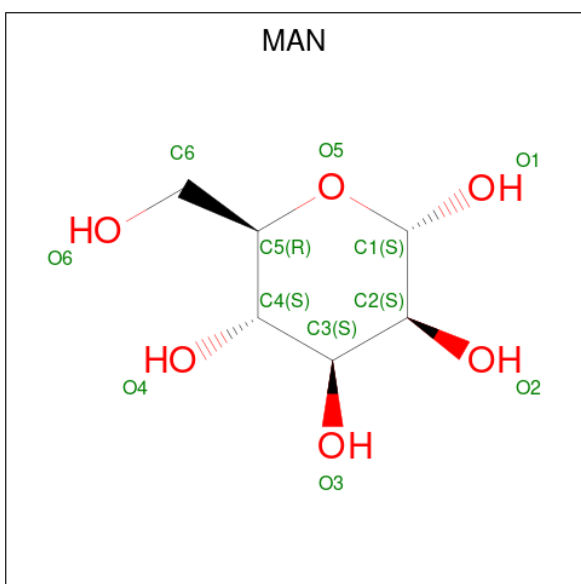
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



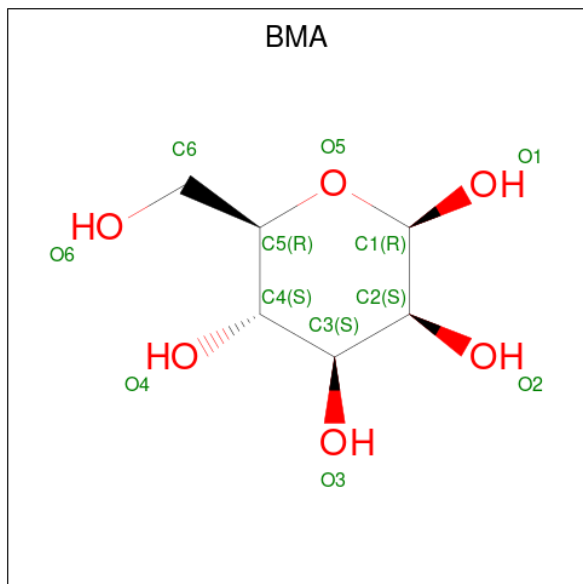
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	H	1	Total	C	O	0	0
			13	8	5		
6	D	1	Total	C	O	0	0
			13	8	5		
6	I	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	12	Total	Ca	0	0
			12	12		
9	D	11	Total	Ca	0	0
			11	11		
9	M	1	Total	Ca	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	81	Total	O	0	0
			81	81		
10	H	76	Total	O	0	0
			76	76		
10	L	107	Total	O	0	0
			107	107		
10	D	62	Total	O	0	0
			62	62		
10	I	103	Total	O	0	0
			103	103		
10	M	105	Total	O	0	0
			105	105		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.34Å 131.62Å 201.76Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	49.54 – 2.95 49.54 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-2.95) 95.6 (49.54-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20rc3-4406	Depositor
R, R_{free}	0.182 , 0.208 0.182 , 0.206	Depositor DCC
R_{free} test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14687	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: NAG, MAN, BMA, EDO, PG4, CA

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	C	0.12	0/4181	0.31	0/5745
1	D	0.09	0/3121	0.24	0/4293
2	H	0.10	0/1701	0.29	0/2328
2	I	0.12	0/1707	0.33	0/2334
3	L	0.11	0/1752	0.31	0/2376
3	M	0.12	0/1755	0.31	0/2379
All	All	0.11	0/14217	0.30	0/19455

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	C	4093	0	3897	46	0
1	D	3068	0	2794	24	0
2	H	1643	0	1596	11	0
2	I	1646	0	1602	15	0
3	L	1703	0	1633	10	0
3	M	1712	0	1650	13	0
4	C	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	8	0	10	0	0
4	I	8	0	12	0	0
5	C	14	0	13	0	0
6	C	26	0	36	3	0
6	D	13	0	18	0	0
6	H	13	0	18	0	0
6	I	13	0	18	3	0
7	C	33	0	30	0	0
8	C	66	0	60	0	0
8	D	66	0	60	1	0
9	C	12	0	0	0	0
9	D	11	0	0	0	0
9	M	1	0	0	0	0
10	C	81	0	0	0	0
10	D	62	0	0	0	0
10	H	76	0	0	0	0
10	I	103	0	0	0	0
10	L	107	0	0	0	0
10	M	105	0	0	0	0
All	All	14687	0	13453	116	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 (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:SER:HB3	1:C:471:PRO:HD2	1.51	0.91
3:M:13:MET:HG3	3:M:19:VAL:HG22	1.71	0.72
1:C:441:PRO:HD3	1:C:524:VAL:HG21	1.76	0.67
1:C:501:LYS:HG3	6:C:604:PG4:H52	1.79	0.64
3:L:13:MET:HG3	3:L:19:VAL:HG22	1.80	0.64
2:I:66:ARG:NH2	2:I:89:ASP:OD2	2.25	0.63
2:I:18:LEU:HB2	2:I:85:LEU:HD11	1.80	0.63
1:C:181:ARG:NH1	1:C:182:GLU:OE2	2.32	0.63
1:C:310:VAL:HG12	1:C:311:SER:H	1.63	0.62
1:C:231:PRO:HA	1:C:324:LEU:HB2	1.82	0.61
1:D:7:ILE:HB	1:D:96:ILE:HD13	1.81	0.61
3:M:201:GLU:HG2	3:M:212:VAL:HG22	1.83	0.60
1:C:7:ILE:HB	1:C:96:ILE:HD13	1.83	0.60
1:C:74:TYR:HB2	1:C:96:ILE:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:TYR:HB2	1:C:321:VAL:HB	1.84	0.59
1:C:499:LYS:HE3	6:C:604:PG4:H21	1.84	0.59
1:D:74:TYR:HB2	1:D:96:ILE:HB	1.84	0.59
1:D:293:LYS:NZ	1:D:295:GLN:O	2.36	0.58
1:C:443:PRO:HD2	1:C:458:ILE:HG23	1.85	0.56
6:I:303:PG4:H22	3:M:104:PHE:H	1.70	0.56
1:D:246:ASP:HB3	1:D:255:TRP:CD1	2.41	0.55
6:I:303:PG4:H22	3:M:104:PHE:HB2	1.88	0.55
1:C:246:ASP:HB3	1:C:255:TRP:CD1	2.42	0.55
1:C:485:THR:HG21	6:C:604:PG4:H31	1.87	0.55
1:C:181:ARG:NH1	1:C:213:ASP:OD1	2.40	0.55
2:I:1:GLN:OE1	2:I:1:GLN:N	2.36	0.55
2:I:11:LEU:HB2	2:I:153:PRO:HG3	1.89	0.54
1:C:372:TRP:HB2	1:C:412:ILE:HG23	1.90	0.54
1:C:293:LYS:NZ	1:C:295:GLN:O	2.39	0.54
1:D:231:PRO:HA	1:D:324:LEU:HB2	1.89	0.53
3:L:201:GLU:HG2	3:L:212:VAL:HG22	1.90	0.53
1:C:441:PRO:HG3	1:C:513:LEU:HD23	1.90	0.52
1:C:517:ASP:OD1	1:C:518:ASN:N	2.35	0.52
1:D:181:ARG:HD3	1:D:213:ASP:HB2	1.91	0.52
1:D:249:ALA:O	1:D:252:THR:OG1	2.24	0.51
1:D:350:GLU:HA	1:D:389:SER:HA	1.93	0.51
2:I:102:LEU:HD22	3:M:55:TYR:CE2	2.46	0.50
1:C:263:ASN:HD21	1:C:298:LEU:HA	1.76	0.50
2:H:165:LEU:HD13	2:H:187:VAL:HG21	1.93	0.50
3:M:181:MET:HE1	3:M:183:SER:HB2	1.93	0.50
2:H:141:MET:HE2	2:H:188:THR:HG22	1.93	0.50
2:I:141:MET:HE3	2:I:188:THR:HG22	1.94	0.50
1:C:10:PRO:HA	1:C:99:THR:HB	1.94	0.49
1:C:442:GLU:HB3	1:C:443:PRO:HD3	1.94	0.49
1:D:118:MET:HA	1:D:212:THR:HB	1.93	0.49
1:D:222:ASN:HB3	1:D:223:PRO:HD3	1.95	0.49
3:M:21:MET:HG2	3:M:108:THR:HG21	1.95	0.49
3:M:142:LEU:HD13	3:M:181:MET:HE2	1.94	0.49
3:L:21:MET:HG2	3:L:108:THR:HG21	1.93	0.49
1:D:159:ASP:HB3	1:D:162:MET:HG2	1.95	0.49
1:C:511:ILE:HD12	1:C:529:VAL:HG21	1.96	0.48
2:I:24:VAL:HG21	2:I:29:LEU:HD13	1.95	0.48
1:C:462:ASP:HB3	1:C:469:THR:HG22	1.96	0.48
3:M:169:TRP:CE2	3:M:181:MET:HG3	2.49	0.48
1:D:105:LYS:HG2	1:D:201:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:SER:HA	1:C:432:SER:HB2	1.97	0.47
1:C:479:GLY:C	1:C:481:SER:H	2.22	0.47
2:I:90:THR:HG23	2:I:116:THR:HA	1.97	0.47
2:H:160:TRP:CZ3	2:H:201:CYS:HB3	2.49	0.47
1:C:105:LYS:HG2	1:C:201:LEU:HB3	1.96	0.46
2:H:82:MET:HB3	2:H:85:LEU:HD11	1.98	0.46
2:H:137:GLN:HG3	2:H:142:VAL:HB	1.97	0.46
3:M:53:LEU:HD21	3:M:68:PHE:CD1	2.49	0.46
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.98	0.46
3:L:41:TRP:CE2	3:L:79:LEU:HB2	2.50	0.46
1:C:222:ASN:HB3	1:C:223:PRO:HD3	1.98	0.46
2:I:165:LEU:HD13	2:I:187:VAL:HG21	1.97	0.46
2:I:38:ARG:HB3	2:I:48:LEU:HD11	1.98	0.45
1:C:470:SER:HB3	1:C:471:PRO:CD	2.36	0.45
1:C:232:GLU:HG3	1:C:290:PHE:H	1.81	0.45
1:C:404:ASN:OD1	1:C:405:SER:N	2.44	0.45
1:C:249:ALA:O	1:C:252:THR:OG1	2.30	0.44
2:I:51:MET:HE3	2:I:71:LYS:HG2	2.00	0.44
1:C:418:SER:HB3	1:C:419:PRO:HD3	1.98	0.44
3:L:156:ILE:HD11	3:L:185:LEU:HD21	1.99	0.44
1:D:223:PRO:HD3	1:D:243:LYS:HB2	1.99	0.44
2:H:18:LEU:HD21	2:H:20:ILE:HD11	2.00	0.44
1:D:352:THR:OG1	1:D:353:SER:N	2.51	0.44
1:C:396:ARG:NH1	1:C:397:GLU:OE2	2.51	0.44
3:M:41:TRP:CE2	3:M:79:LEU:HB2	2.53	0.44
3:L:155:LYS:HB2	3:L:199:THR:HB	2.00	0.43
3:L:112:ILE:O	3:L:172:GLN:NE2	2.40	0.43
1:D:14:LYS:HB2	3:M:99[B]:ARG:HG2	2.00	0.43
1:D:156:GLU:HB2	1:D:160:LYS:HA	2.00	0.43
1:D:229:GLN:HG2	1:D:322:ASP:HB2	2.01	0.43
2:I:160:TRP:CZ3	2:I:201:CYS:HB3	2.54	0.43
1:C:223:PRO:HD2	1:C:226:TYR:OH	2.19	0.43
1:C:298:LEU:HB2	1:C:319:VAL:HG13	2.00	0.43
1:C:446:ILE:HG23	1:C:456:GLN:HG2	2.01	0.43
1:D:68:ARG:HD3	1:D:100:ASP:HB2	2.01	0.42
1:C:484:TRP:CE2	1:C:511:ILE:HD11	2.54	0.42
3:L:53:LEU:HD21	3:L:68:PHE:CD1	2.54	0.42
1:D:255:TRP:CH2	1:D:278:ASN:HB2	2.54	0.42
1:C:388:ILE:HD13	1:C:427:LEU:HD22	2.00	0.42
3:L:195:HIS:O	3:L:217:ARG:HD3	2.19	0.42
1:D:113:PHE:CG	1:D:130:VAL:HG12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:67:LEU:HD22	2:I:80:LEU:HD11	2.02	0.42
2:H:38:ARG:HB3	2:H:48:LEU:HD11	2.02	0.41
2:H:221:CYS:HB3	2:H:222:HIS:H	1.68	0.41
1:C:29:ASP:HA	1:C:32:GLY:O	2.20	0.41
1:D:154:ASP:HA	1:D:155:PRO:HA	1.89	0.41
2:I:47:TRP:H	6:I:303:PG4:H21	1.85	0.41
2:I:102:LEU:HD22	3:M:55:TYR:CZ	2.56	0.41
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.56	0.41
1:D:234:GLU:HB3	1:D:237:VAL:HG21	2.03	0.41
1:D:171:VAL:HG11	8:D:606:BMA:H62	2.03	0.41
1:C:218:PRO:HA	1:C:219:PRO:HD3	1.99	0.40
1:C:26:SER:OG	1:C:89:GLU:OE2	2.30	0.40
1:C:402:VAL:HG12	1:C:404:ASN:O	2.21	0.40
2:H:67:LEU:HD22	2:H:80:LEU:HD11	2.02	0.40
1:C:159:ASP:OD1	1:C:160:LYS:N	2.54	0.40
1:C:371:ILE:HG12	1:C:381:ILE:HG22	2.02	0.40
3:L:41:TRP:HB2	3:L:54:ILE:HB	2.03	0.40
1:C:154:ASP:HA	1:C:155:PRO:HA	1.82	0.40
1:C:223:PRO:HD3	1:C:243:LYS:HB2	2.04	0.40
1:D:298:LEU:HB2	1:D:319:VAL:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	539/590 (91%)	504 (94%)	30 (6%)	5 (1%)	14	34
1	D	410/590 (70%)	387 (94%)	23 (6%)	0	100	100
2	H	220/246 (89%)	213 (97%)	7 (3%)	0	100	100
2	I	218/246 (89%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
3	M	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
All	All	1827/2152 (85%)	1751 (96%)	71 (4%)	5 (0%)	36	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	310	VAL
1	C	471	PRO
1	C	472	PHE
1	C	232	GLU
1	C	419	PRO

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	C	455/507 (90%)	445 (98%)	10 (2%)	45	69
1	D	323/507 (64%)	313 (97%)	10 (3%)	35	59
2	H	188/214 (88%)	186 (99%)	2 (1%)	65	80
2	I	189/214 (88%)	186 (98%)	3 (2%)	55	75
3	L	196/214 (92%)	194 (99%)	2 (1%)	68	82
3	M	196/214 (92%)	193 (98%)	3 (2%)	57	76
All	All	1547/1870 (83%)	1517 (98%)	30 (2%)	51	71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	GLU
1	C	206	THR
1	C	310	VAL
1	C	319	VAL
1	C	341	VAL

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Mol	Chain	Res	Type
1	C	358	GLU
1	C	396	ARG
1	C	456	GLN
1	C	478	HIS
1	C	485	THR
2	H	58[A]	ASP
2	H	58[B]	ASP
3	L	181	MET
3	L	187	LEU
1	D	81	VAL
1	D	111	GLU
1	D	119	GLU
1	D	199	GLU
1	D	206	THR
1	D	258	VAL
1	D	271	VAL
1	D	306	VAL
1	D	319	VAL
1	D	358	GLU
2	I	58[A]	ASP
2	I	58[B]	ASP
2	I	165	LEU
3	M	129	GLU
3	M	151	ASN
3	M	181	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	197	GLN
1	C	217	ASN
1	C	236	ASN
1	C	268	GLN
1	C	437	ASN
2	H	16	GLN
2	H	77	GLN
2	H	86	GLN
3	L	43	GLN
3	L	102	HIS
3	L	151	ASN
1	D	217	ASN
1	D	233	ASN

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Mol	Chain	Res	Type
1	D	251	ASN
1	D	294	GLN
1	D	295	GLN
1	D	401	HIS
1	D	437	ASN
2	I	56	ASN
2	I	86	GLN
3	M	37	ASN

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 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 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	$\# Z > 2$
8	BMA	C	610	-	11,11,12	0.72	0	15,15,17	0.99	2 (13%)
4	EDO	I	301	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	H	301	-	3,3,3	0.45	0	2,2,2	0.33	0
4	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	C	601	-	3,3,3	0.47	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	D	603	-	11,11,12	0.81	0	15,15,17	1.26	2 (13%)
8	BMA	D	602	-	11,11,12	0.76	0	15,15,17	0.95	1 (6%)
6	PG4	H	303	-	12,12,12	0.14	0	11,11,11	0.62	0
8	BMA	D	606	-	11,11,12	0.82	0	15,15,17	1.12	2 (13%)
8	BMA	C	612	-	11,11,12	0.85	0	15,15,17	1.49	2 (13%)
8	BMA	C	613	-	11,11,12	0.82	0	15,15,17	1.28	2 (13%)
4	EDO	I	302	-	3,3,3	0.44	0	2,2,2	0.34	0
8	BMA	C	608	-	11,11,12	0.73	0	15,15,17	1.31	2 (13%)
8	BMA	D	605	-	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
5	NAG	C	602	1	14,14,15	0.28	0	17,19,21	0.45	0
6	PG4	C	603	-	12,12,12	0.12	0	11,11,11	0.61	0
7	MAN	C	607	1	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
7	MAN	C	605	1	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
8	BMA	D	607	-	11,11,12	0.82	0	15,15,17	1.34	2 (13%)
6	PG4	C	604	-	12,12,12	0.14	0	11,11,11	0.61	0
6	PG4	D	601	-	12,12,12	0.13	0	11,11,11	0.61	0
6	PG4	I	303	-	12,12,12	0.12	0	11,11,11	0.65	0
7	MAN	C	611	1	11,11,12	0.75	0	15,15,17	1.16	2 (13%)
8	BMA	D	604	-	11,11,12	0.65	0	15,15,17	1.03	2 (13%)
8	BMA	C	606	-	11,11,12	0.89	1 (9%)	15,15,17	0.98	2 (13%)
8	BMA	C	609	-	11,11,12	0.91	0	15,15,17	1.18	2 (13%)

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
8	BMA	C	610	-	-	2/2/19/22	0/1/1/1
4	EDO	I	301	-	-	0/1/1/1	-
4	EDO	H	301	-	-	0/1/1/1	-
4	EDO	H	302	-	-	0/1/1/1	-
4	EDO	C	601	-	-	0/1/1/1	-
8	BMA	D	603	-	-	0/2/19/22	1/1/1/1
8	BMA	D	602	-	-	0/2/19/22	0/1/1/1
6	PG4	H	303	-	-	6/10/10/10	-
8	BMA	D	606	-	-	2/2/19/22	0/1/1/1
8	BMA	C	612	-	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	C	613	-	-	1/2/19/22	0/1/1/1
4	EDO	I	302	-	-	0/1/1/1	-
8	BMA	C	608	-	-	2/2/19/22	0/1/1/1
8	BMA	D	605	-	-	0/2/19/22	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
6	PG4	C	603	-	-	2/10/10/10	-
7	MAN	C	607	1	-	2/2/19/22	0/1/1/1
7	MAN	C	605	1	-	0/2/19/22	0/1/1/1
8	BMA	D	607	-	-	1/2/19/22	0/1/1/1
6	PG4	C	604	-	-	3/10/10/10	-
6	PG4	D	601	-	-	5/10/10/10	-
6	PG4	I	303	-	-	8/10/10/10	-
7	MAN	C	611	1	-	0/2/19/22	0/1/1/1
8	BMA	D	604	-	-	2/2/19/22	0/1/1/1
8	BMA	C	606	-	-	2/2/19/22	0/1/1/1
8	BMA	C	609	-	-	2/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	606	BMA	O5-C1	-2.11	1.40	1.43

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	612	BMA	C1-O5-C5	4.30	117.94	112.19
8	D	607	BMA	C1-O5-C5	3.85	117.35	112.19
8	C	608	BMA	C1-O5-C5	3.80	117.27	112.19
8	D	603	BMA	C1-O5-C5	3.77	117.23	112.19
8	C	613	BMA	C1-O5-C5	3.66	117.09	112.19
8	C	609	BMA	C1-O5-C5	3.24	116.53	112.19
7	C	611	MAN	C1-O5-C5	3.12	116.37	112.19
8	D	604	BMA	C1-O5-C5	2.49	115.52	112.19
8	D	606	BMA	C1-O5-C5	2.46	115.48	112.19
7	C	607	MAN	C1-O5-C5	2.45	115.47	112.19
8	D	605	BMA	C1-O5-C5	2.43	115.44	112.19
8	C	610	BMA	C1-O5-C5	2.30	115.28	112.19
7	C	605	MAN	C1-O5-C5	2.25	115.20	112.19
8	D	606	BMA	O2-C2-C3	-2.24	105.51	110.15
8	C	609	BMA	O2-C2-C3	-2.23	105.53	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	605	BMA	O2-C2-C3	-2.21	105.56	110.15
8	D	602	BMA	C1-O5-C5	2.20	115.13	112.19
8	C	608	BMA	O2-C2-C3	-2.20	105.60	110.15
8	D	603	BMA	O2-C2-C3	-2.14	105.71	110.15
8	C	612	BMA	O2-C2-C3	-2.14	105.72	110.15
8	C	606	BMA	O2-C2-C3	-2.13	105.75	110.15
8	C	610	BMA	O2-C2-C3	-2.11	105.77	110.15
8	D	604	BMA	O2-C2-C3	-2.10	105.80	110.15
7	C	611	MAN	O2-C2-C3	-2.10	105.81	110.15
7	C	607	MAN	O2-C2-C3	-2.09	105.81	110.15
8	D	607	BMA	O2-C2-C3	-2.09	105.82	110.15
8	C	613	BMA	O2-C2-C3	-2.08	105.85	110.15
8	C	606	BMA	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	612	BMA	O5-C5-C6-O6
8	C	608	BMA	O5-C5-C6-O6
7	C	607	MAN	O5-C5-C6-O6
8	C	609	BMA	C4-C5-C6-O6
7	C	607	MAN	C4-C5-C6-O6
8	D	604	BMA	C4-C5-C6-O6
5	C	602	NAG	C8-C7-N2-C2
5	C	602	NAG	O7-C7-N2-C2
8	C	606	BMA	O5-C5-C6-O6
8	C	609	BMA	O5-C5-C6-O6
8	D	604	BMA	O5-C5-C6-O6
8	C	612	BMA	C4-C5-C6-O6
8	C	608	BMA	C4-C5-C6-O6
8	D	606	BMA	O5-C5-C6-O6
8	C	613	BMA	O5-C5-C6-O6
6	C	604	PG4	O2-C3-C4-O3
6	H	303	PG4	O4-C7-C8-O5
6	I	303	PG4	O4-C7-C8-O5
6	D	601	PG4	O3-C5-C6-O4
6	H	303	PG4	O2-C3-C4-O3
8	D	607	BMA	O5-C5-C6-O6
6	C	603	PG4	O2-C3-C4-O3
8	C	610	BMA	C4-C5-C6-O6
8	C	606	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	C	604	PG4	C5-C6-O4-C7
6	H	303	PG4	C3-C4-O3-C5
6	D	601	PG4	C3-C4-O3-C5
6	I	303	PG4	C4-C3-O2-C2
6	C	604	PG4	C6-C5-O3-C4
6	H	303	PG4	C4-C3-O2-C2
6	D	601	PG4	C6-C5-O3-C4
6	I	303	PG4	C8-C7-O4-C6
6	I	303	PG4	C3-C4-O3-C5
6	I	303	PG4	C6-C5-O3-C4
6	D	601	PG4	O2-C3-C4-O3
8	D	606	BMA	C4-C5-C6-O6
6	C	603	PG4	C4-C3-O2-C2
8	C	610	BMA	O5-C5-C6-O6
6	I	303	PG4	O2-C3-C4-O3
6	H	303	PG4	O1-C1-C2-O2
6	I	303	PG4	C1-C2-O2-C3
6	H	303	PG4	C6-C5-O3-C4
6	I	303	PG4	O1-C1-C2-O2
6	D	601	PG4	C4-C3-O2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	609	BMA	C1-C2-C3-C4-C5-O5
8	D	603	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	606	BMA	1	0
6	C	604	PG4	3	0
6	I	303	PG4	3	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	C	540/590 (91%)	0.52	50 (9%) 14 12	35, 99, 146, 213	1 (0%)
1	D	422/590 (71%)	1.00	92 (21%) 2 2	36, 134, 179, 224	0
2	H	219/246 (89%)	0.04	14 (6%) 25 21	23, 60, 131, 179	5 (2%)
2	I	216/246 (87%)	-0.20	8 (3%) 45 37	22, 46, 82, 182	6 (2%)
3	L	220/240 (91%)	-0.18	3 (1%) 73 67	28, 52, 96, 154	2 (0%)
3	M	220/240 (91%)	-0.37	2 (0%) 81 76	25, 46, 85, 140	2 (0%)
All	All	1837/2152 (85%)	0.30	169 (9%) 14 13	22, 65, 161, 224	16 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	526	THR	7.8
1	D	157	LEU	6.8
1	C	470	SER	6.2
3	M	220	CYS	6.1
1	C	540	VAL	5.7
1	C	525	THR	5.7
2	H	136	ALA	5.6
1	D	420	VAL	5.4
1	D	423	GLY	5.2
2	H	139	ASN	5.2
2	H	222	HIS	5.1
2	I	138	THR	4.9
2	I	137	GLN	4.9
1	D	300	VAL	4.8
1	D	362	PHE	4.7
1	D	342	SER	4.6
1	C	417	GLY	4.6
1	C	420	VAL	4.4
1	D	405	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	344	ASP	4.2
2	I	140	SER	4.2
1	D	309	GLU	4.2
1	D	354	TYR	4.2
1	D	372	TRP	4.1
1	C	361	THR	4.1
1	D	325	ASP	4.0
2	H	220	ASP	3.9
2	H	138	THR	3.8
1	C	372	TRP	3.7
1	D	422	THR	3.7
1	D	401	HIS	3.7
2	H	137	GLN	3.7
1	D	391	ARG	3.7
1	C	399	PHE	3.7
3	L	218	ASN	3.6
1	C	418	SER	3.6
3	L	220	CYS	3.5
1	D	339	VAL	3.5
1	D	435	ASN	3.4
2	I	220	ASP	3.4
1	D	398	ASP	3.4
1	D	341	VAL	3.3
1	D	373	ARG	3.3
1	D	412	ILE	3.3
1	D	158	PRO	3.3
1	D	269	PHE	3.2
1	C	442	GLU	3.2
1	D	281	ILE	3.2
1	C	370	ARG	3.2
1	C	423	GLY	3.1
1	D	231	PRO	3.1
1	C	424	THR	3.1
1	D	368	THR	3.1
1	D	308	PHE	3.1
1	C	405	SER	3.1
1	D	287	GLY	3.0
2	H	219	ARG	3.0
1	C	186	THR	3.0
1	D	346	GLY	3.0
1	C	363	MET	3.0
1	D	245	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	383	PRO	2.9
2	H	195	PRO	2.9
1	D	329	ALA	2.9
1	D	337	LYS	2.9
1	D	239	ILE	2.9
1	C	419	PRO	2.9
1	D	404	ASN	2.9
1	D	241	THR	2.9
1	D	352	THR	2.8
1	D	335	PRO	2.8
1	D	327	ASN	2.8
1	C	123	PRO	2.8
2	H	132	PRO	2.8
1	C	247	ALA	2.7
1	D	345	PHE	2.7
1	D	356	ALA	2.7
1	C	312	LEU	2.7
1	D	324	LEU	2.7
1	D	331	ILE	2.7
1	D	408	THR	2.7
1	D	349	GLN	2.7
1	C	118	MET	2.7
1	D	187	TYR	2.7
1	D	353	SER	2.7
1	D	351	ILE	2.7
2	H	196	SER	2.7
1	C	313	THR	2.6
1	D	176	THR	2.6
1	C	408	THR	2.6
1	D	303	THR	2.6
1	D	298	LEU	2.6
1	C	519	GLN	2.6
1	D	111	GLU	2.6
1	D	350	GLU	2.6
1	C	362	PHE	2.6
1	D	406	THR	2.6
1	D	380	GLU	2.6
1	C	471	PRO	2.6
1	D	286	LYS	2.6
1	D	348	GLY	2.6
1	D	436	ASP	2.5
1	C	393	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	429	LEU	2.5
1	D	275	PRO	2.5
1	D	326	VAL	2.5
1	C	364	GLU	2.5
1	D	407	TYR	2.5
1	D	320	THR	2.5
1	D	366	LYS	2.5
1	D	276	VAL	2.4
1	D	225	THR	2.4
1	D	263	ASN	2.4
1	D	220	ILE	2.4
1	C	178	GLY	2.4
2	I	192	SER	2.4
1	C	241	THR	2.4
1	C	122	LEU	2.4
1	C	342	SER	2.4
1	D	378	TRP	2.4
1	C	226	TYR	2.4
1	C	413	ALA	2.4
1	C	158	PRO	2.4
1	C	311	SER	2.3
1	D	403	LYS	2.3
1	D	122	LEU	2.3
1	C	366	LYS	2.3
2	H	193	PRO	2.3
1	D	299	HIS	2.3
1	D	424	THR	2.3
1	C	310	VAL	2.3
2	I	139	ASN	2.3
1	D	296	TYR	2.3
1	D	347	VAL	2.3
1	D	118	MET	2.2
1	D	437	ASN	2.2
1	D	224	THR	2.2
1	D	434	VAL	2.2
1	C	416	ASN	2.2
1	C	391	ARG	2.2
1	D	402	VAL	2.2
1	C	179	LEU	2.2
1	D	413	ALA	2.2
2	H	194	ARG	2.2
1	C	435	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	502	MET	2.2
1	C	231	PRO	2.1
1	D	270	VAL	2.1
1	D	178	GLY	2.1
1	C	392	ALA	2.1
1	C	520	ASN	2.1
3	L	163	ASN	2.1
1	C	333	VAL	2.1
1	D	33	LYS	2.1
1	D	113	PHE	2.1
1	D	247	ALA	2.1
1	C	309	GLU	2.1
3	M	219	GLU	2.1
1	D	152	SER	2.1
1	D	183	SER	2.1
2	H	192	SER	2.1
2	H	1	GLN	2.1
1	D	223	PRO	2.1
2	I	191	SER	2.0
1	C	469	THR	2.0
1	D	414	THR	2.0
2	I	219	ARG	2.0
1	D	367	ILE	2.0
1	D	336	GLU	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($\text{\AA}^2$)	Q<0.9
8	BMA	D	604	11/12	0.51	0.19	153,158,171,176	0
8	BMA	D	605	11/12	0.51	0.19	123,156,166,171	0
8	BMA	D	602	11/12	0.68	0.26	85,124,137,143	0
8	BMA	C	612	11/12	0.69	0.17	122,132,143,145	0
7	MAN	C	607	11/12	0.69	0.20	135,156,174,174	0
8	BMA	C	609	11/12	0.71	0.18	109,122,141,152	0
8	BMA	C	608	11/12	0.73	0.14	130,134,146,148	0
9	CA	D	615	1/1	0.73	0.09	159,159,159,159	0
8	BMA	D	607	11/12	0.75	0.11	130,149,159,160	0
7	MAN	C	605	11/12	0.76	0.17	93,109,117,123	0
5	NAG	C	602	14/15	0.76	0.23	78,111,123,125	0
6	PG4	C	604	13/13	0.77	0.27	66,84,102,105	0
7	MAN	C	611	11/12	0.78	0.18	96,122,130,141	0
8	BMA	D	606	11/12	0.79	0.14	127,135,144,147	0
8	BMA	D	603	11/12	0.80	0.18	99,120,129,136	0
8	BMA	C	613	11/12	0.81	0.14	112,128,153,160	0
8	BMA	C	606	11/12	0.83	0.14	93,109,133,136	0
4	EDO	H	302	4/4	0.83	0.27	105,108,110,142	0
8	BMA	C	610	11/12	0.84	0.16	133,147,151,152	0
6	PG4	C	603	13/13	0.84	0.18	80,94,116,137	0
9	CA	C	622	1/1	0.85	0.13	106,106,106,106	0
6	PG4	D	601	13/13	0.86	0.18	76,88,101,117	0
4	EDO	C	601	4/4	0.86	0.24	60,70,73,87	0
9	CA	M	301	1/1	0.88	0.22	99,99,99,99	0
9	CA	D	608	1/1	0.90	0.09	173,173,173,173	0
9	CA	D	610	1/1	0.90	0.08	152,152,152,152	0
6	PG4	H	303	13/13	0.90	0.19	24,85,105,107	0
4	EDO	H	301	4/4	0.90	0.13	66,67,75,76	0
4	EDO	I	302	4/4	0.91	0.19	70,75,75,79	0
4	EDO	I	301	4/4	0.92	0.12	48,48,55,62	0
6	PG4	I	303	13/13	0.92	0.20	5,76,106,121	0
9	CA	D	617	1/1	0.93	0.15	169,169,169,169	0
9	CA	C	625	1/1	0.93	0.09	133,133,133,133	0
9	CA	D	618	1/1	0.95	0.07	207,207,207,207	0
9	CA	D	616	1/1	0.96	0.06	124,124,124,124	0
9	CA	C	624	1/1	0.96	0.10	116,116,116,116	0
9	CA	D	614	1/1	0.97	0.06	135,135,135,135	0
9	CA	C	615	1/1	0.97	0.10	53,53,53,53	0
9	CA	C	618	1/1	0.98	0.05	118,118,118,118	0
9	CA	C	619	1/1	0.98	0.06	135,135,135,135	0
9	CA	C	617	1/1	0.98	0.04	109,109,109,109	0
9	CA	D	609	1/1	0.98	0.04	135,135,135,135	0
9	CA	C	623	1/1	0.98	0.06	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CA	D	611	1/1	0.98	0.12	49,49,49,49	0
9	CA	C	620	1/1	0.99	0.04	73,73,73,73	0
9	CA	C	621	1/1	0.99	0.04	87,87,87,87	0
9	CA	D	613	1/1	0.99	0.06	53,53,53,53	0
9	CA	C	614	1/1	1.00	0.03	43,43,43,43	0
9	CA	D	612	1/1	1.00	0.02	44,44,44,44	0
9	CA	C	616	1/1	1.00	0.01	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.