



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:10 AM BST

PDB ID : 3C09
Title : Crystal structure the Fab fragment of matuzumab (Fab72000) in complex with domain III of the extracellular region of EGFR
Authors : Ferguson, K.M.; Schmiedel, J.; Knoechel, T.
Deposited on : 2008-01-18
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

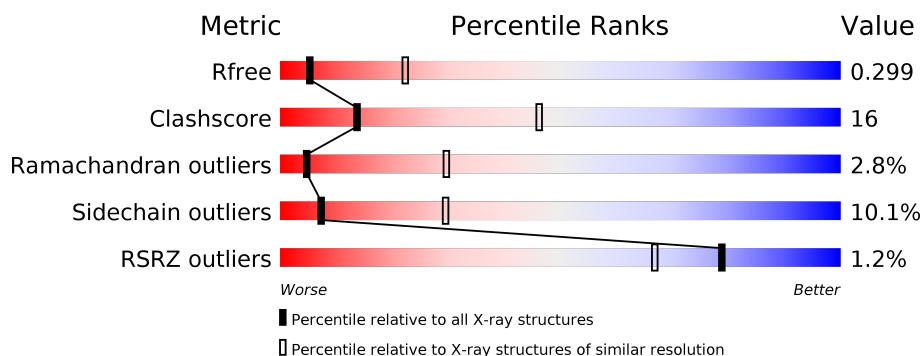
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	B	212	<p>2% 54% 26% 17%</p>
1	L	212	<p>71% 27%</p>
2	C	223	<p>4% 61% 20% 14%</p>
2	H	223	<p>66% 27%</p>
3	A	214	<p>58% 27% 11%</p>
3	D	214	<p>62% 26% 11%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	4202	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8532 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 Matuzumab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1533	959	252	316	6			
1	B	175	Total	C	N	O	S	0	0	0
			1239	772	204	258	5			

- Molecule 2 is a protein called Matuzumab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1573	996	259	311	7			
2	C	191	Total	C	N	O	S	0	0	0
			1347	846	224	270	7			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	191	Total	C	N	O	S	0	0	0
			1371	857	237	269	8			
3	D	191	Total	C	N	O	S	0	0	0
			1296	807	226	255	8			

There are 22 discrepancies between the modelled and reference sequences:

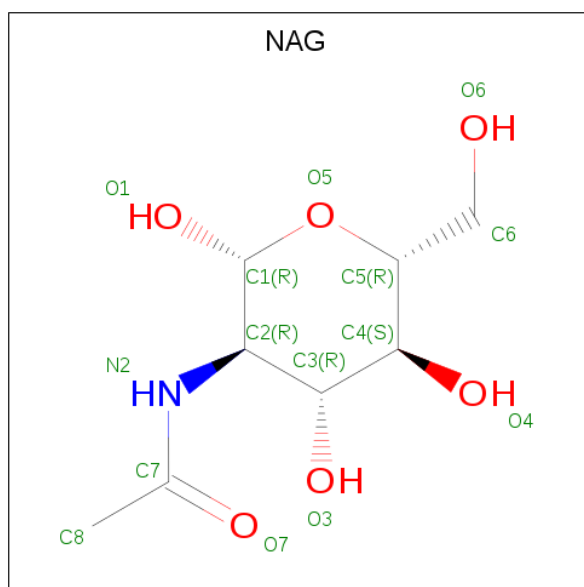
Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	expression tag	UNP P00533
A	308	GLU	-	expression tag	UNP P00533
A	309	GLU	-	expression tag	UNP P00533
A	310	LYS	-	expression tag	UNP P00533
A	311	LYS	-	expression tag	UNP P00533
A	515	HIS	-	expression tag	UNP P00533
A	516	HIS	-	expression tag	UNP P00533
A	517	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
A	518	HIS	-	expression tag	UNP P00533
A	519	HIS	-	expression tag	UNP P00533
A	520	HIS	-	expression tag	UNP P00533
D	307	LEU	-	expression tag	UNP P00533
D	308	GLU	-	expression tag	UNP P00533
D	309	GLU	-	expression tag	UNP P00533
D	310	LYS	-	expression tag	UNP P00533
D	311	LYS	-	expression tag	UNP P00533
D	515	HIS	-	expression tag	UNP P00533
D	516	HIS	-	expression tag	UNP P00533
D	517	HIS	-	expression tag	UNP P00533
D	518	HIS	-	expression tag	UNP P00533
D	519	HIS	-	expression tag	UNP P00533
D	520	HIS	-	expression tag	UNP P00533

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



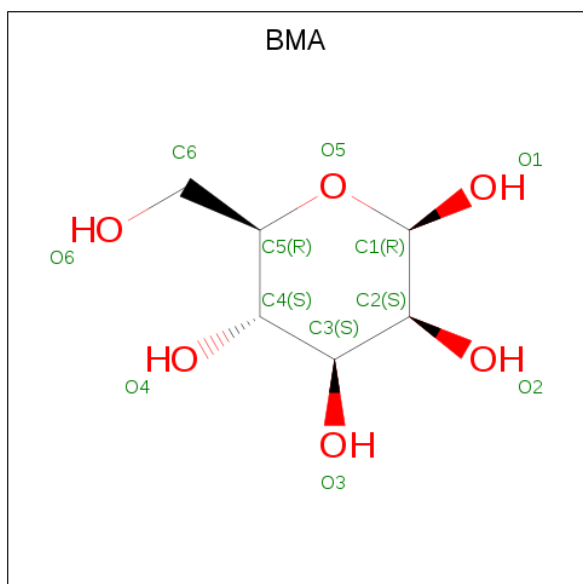
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



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

- Molecule 6 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

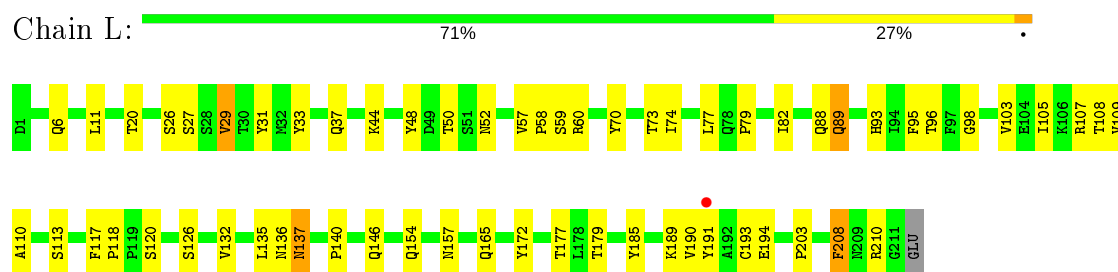


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

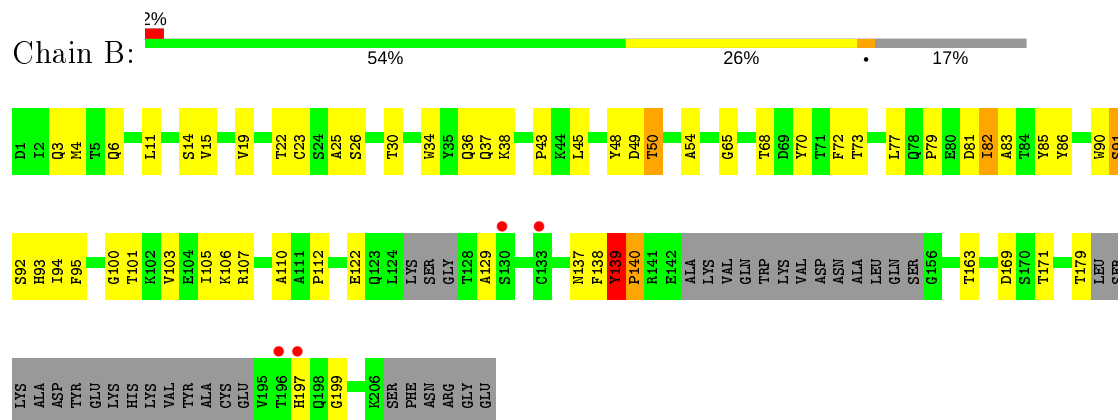
3 Residue-property plots

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.

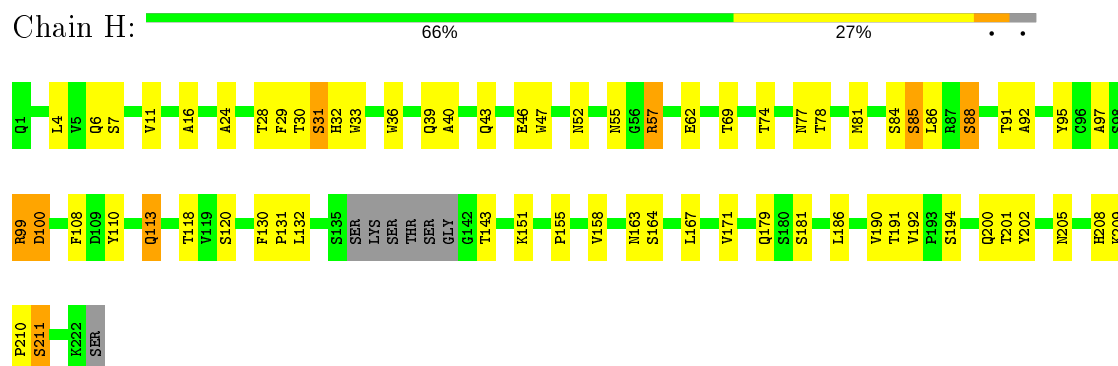
- Molecule 1: Matuzumab Fab Light chain



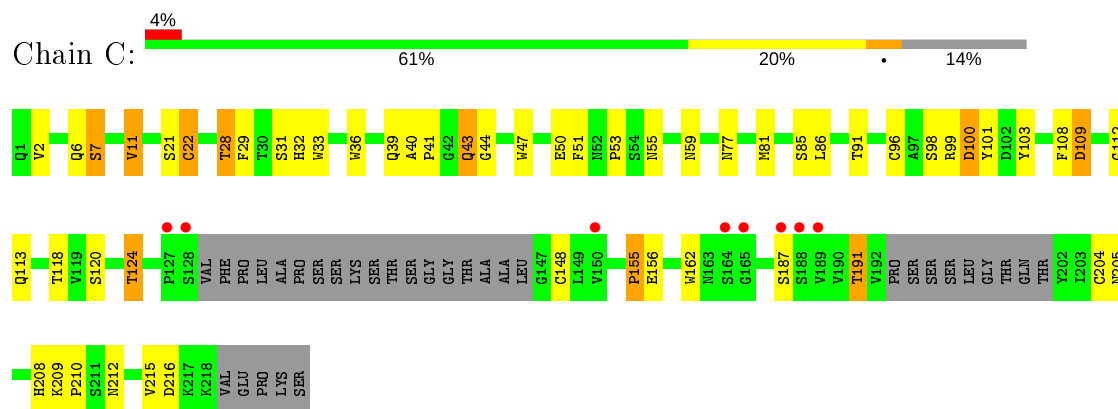
- Molecule 1: Matuzumab Fab Light chain



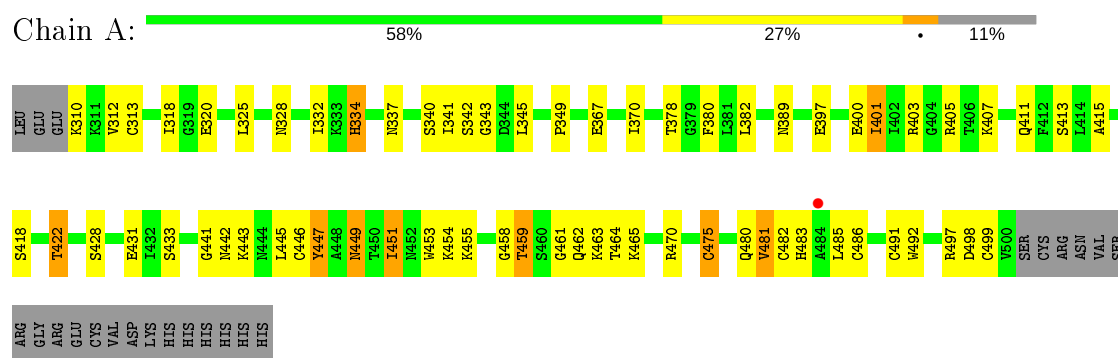
- Molecule 2: Matuzumab Fab Heavy chain



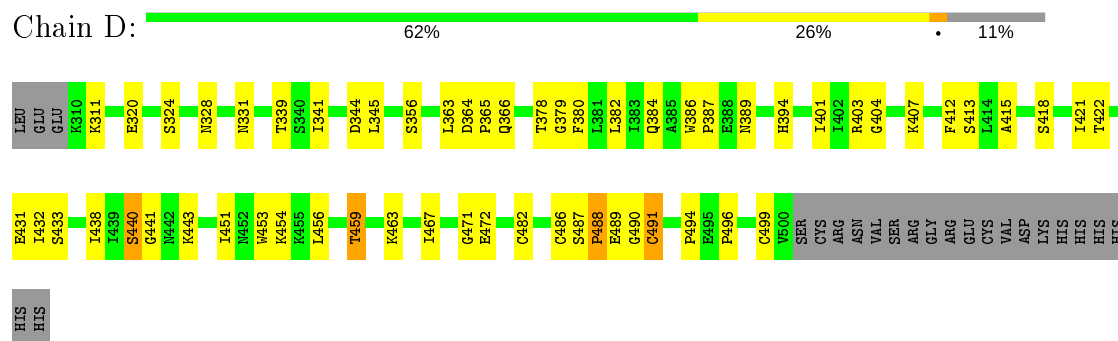
- Molecule 2: Matuzumab Fab Heavy chain



- Molecule 3: Epidermal growth factor receptor



- Molecule 3: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.07Å 205.03Å 81.58Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	36.56 – 3.20 45.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.56-3.20) 99.7 (45.47-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.299 0.240 , 0.299	Depositor DCC
R_{free} test set	1709 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: BMA, NAG, MAN

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	B	0.51	1/1266 (0.1%)	0.66	1/1732 (0.1%)
1	L	0.48	0/1570	0.63	0/2152
2	C	0.49	0/1383	0.63	0/1902
2	H	0.49	0/1616	0.61	0/2223
3	A	0.46	0/1396	0.64	0/1907
3	D	0.46	0/1322	0.60	0/1815
All	All	0.48	1/8553 (0.0%)	0.63	1/11731 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	CYS	CB-SG	-5.02	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	TYR	C-N-CD	-5.46	108.59	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	191	THR	Peptide
2	H	99	ARG	Peptide

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	B	1239	0	1067	56	0
1	L	1533	0	1358	47	0
2	C	1347	0	1109	36	0
2	H	1573	0	1405	39	0
3	A	1371	0	1271	48	0
3	D	1296	0	1101	33	0
4	A	84	0	78	10	0
4	D	56	0	52	4	0
5	A	11	0	10	1	0
5	D	11	0	10	0	0
6	A	11	0	10	1	0
All	All	8532	0	7471	243	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 16.

All (243) 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:B:139:TYR:CD2	1:B:140:PRO:HD3	1.69	1.26
1:B:139:TYR:CG	1:B:140:PRO:HD3	1.74	1.22
1:B:139:TYR:CB	1:B:140:PRO:CD	2.27	1.10
1:B:139:TYR:HB3	1:B:140:PRO:CD	1.82	1.09
1:B:139:TYR:CG	1:B:140:PRO:CD	2.41	1.03
1:L:191:TYR:HB2	1:L:208:PHE:HE1	1.21	1.01
3:A:328:ASN:HD21	4:A:3281:NAG:C1	1.74	1.00
3:D:328:ASN:HD21	4:D:3281:NAG:C1	1.74	1.00
3:A:446:CYS:HG	3:A:475:CYS:HG	1.07	0.99
1:B:139:TYR:HB3	1:B:140:PRO:HD2	1.45	0.97
1:B:139:TYR:CB	1:B:140:PRO:HD3	1.93	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:PRO:HA	1:L:105:ILE:CD1	1.98	0.93
1:L:191:TYR:HB2	1:L:208:PHE:CE1	2.06	0.90
3:D:331:ASN:HB3	4:D:3281:NAG:H61	1.55	0.89
3:A:328:ASN:ND2	4:A:3281:NAG:C1	2.35	0.89
3:A:458:GLY:H	3:A:462:GLN:HE22	1.20	0.88
3:D:382:LEU:HD11	3:D:384:GLN:HE21	1.38	0.88
2:H:32:HIS:HD2	2:H:100:ASP:OD2	1.56	0.88
1:L:118:PRO:HB3	1:L:208:PHE:CE2	2.08	0.87
1:L:146:GLN:HB3	1:L:194:GLU:HG3	1.58	0.85
1:B:30:THR:HG22	1:B:91:SER:HA	1.56	0.85
1:B:139:TYR:CD2	1:B:140:PRO:CD	2.61	0.81
3:A:389:ASN:HD21	4:A:3891:NAG:C1	1.94	0.81
1:B:139:TYR:HB3	1:B:140:PRO:HD3	1.55	0.81
3:D:328:ASN:ND2	4:D:3281:NAG:C1	2.42	0.81
3:A:380:PHE:HB2	3:A:413:SER:HA	1.62	0.80
3:A:482:CYS:HA	3:A:491:CYS:SG	2.22	0.79
2:H:100:ASP:OD2	3:D:454:LYS:HE3	1.84	0.76
3:A:341:ILE:HD13	3:A:345:LEU:HD21	1.68	0.75
1:B:30:THR:CG2	1:B:91:SER:HA	2.16	0.75
1:L:118:PRO:HB3	1:L:208:PHE:HE2	1.53	0.74
3:A:337:ASN:HD21	4:A:3371:NAG:C1	2.02	0.73
1:B:139:TYR:CG	1:B:140:PRO:N	2.54	0.72
3:D:378:THR:O	3:D:403:ARG:HB2	1.90	0.72
2:C:6:GLN:HE22	2:C:96:CYS:H	1.37	0.71
2:H:29:PHE:HB2	2:H:77:ASN:ND2	2.05	0.70
3:D:486:CYS:HG	3:D:499:CYS:HG	0.74	0.70
1:L:146:GLN:HB3	1:L:194:GLU:CG	2.22	0.70
1:L:37:GLN:HE22	2:H:39:GLN:HE22	1.37	0.70
1:B:11:LEU:HD21	1:B:19:VAL:HG13	1.74	0.68
1:B:36:GLN:HG3	1:B:85:TYR:CE2	2.28	0.68
2:H:32:HIS:CD2	2:H:100:ASP:OD2	2.44	0.68
5:A:3283:BMA:H2	6:A:3284:MAN:C1	2.23	0.68
4:D:3281:NAG:O4	4:D:3282:NAG:C1	2.42	0.67
1:L:79:PRO:HA	1:L:105:ILE:HD12	1.75	0.67
3:A:431:GLU:OE2	3:A:433:SER:HB3	1.95	0.66
1:B:45:LEU:HD21	1:B:48:TYR:HB3	1.75	0.66
2:C:33:TRP:HD1	2:C:100:ASP:OD2	1.78	0.66
2:H:151:LYS:CE	2:H:179:GLN:HE22	2.09	0.66
3:A:458:GLY:N	3:A:462:GLN:HE22	1.93	0.65
3:A:422:THR:HG22	3:A:480:GLN:HE22	1.62	0.65
1:B:49:ASP:O	1:B:50:THR:HB	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD12	1:B:81:ASP:HB2	1.79	0.65
3:D:415:ALA:HA	3:D:438:ILE:HG23	1.78	0.63
4:A:3281:NAG:O4	4:A:3282:NAG:C1	2.47	0.63
2:H:6:GLN:HB2	2:H:113:GLN:HE22	1.64	0.63
1:B:77:LEU:CD1	1:B:81:ASP:HB2	2.29	0.62
3:D:341:ILE:HD13	3:D:345:LEU:HD21	1.81	0.62
2:C:99:ARG:HA	2:C:108:PHE:O	1.99	0.62
3:A:418:SER:HA	3:A:441:GLY:O	2.00	0.62
2:H:151:LYS:HE3	2:H:179:GLN:HE22	1.64	0.62
1:L:37:GLN:NE2	2:H:39:GLN:HE22	1.98	0.62
2:H:167:LEU:HD21	2:H:190:VAL:HG11	1.82	0.62
3:D:432:ILE:HD12	3:D:456:LEU:HD22	1.82	0.61
1:L:79:PRO:HA	1:L:105:ILE:HD11	1.83	0.61
1:B:34:TRP:CE2	1:B:72:PHE:HB2	2.35	0.61
3:A:332:ILE:HG13	3:A:370:ILE:HD12	1.83	0.61
2:C:40:ALA:O	2:C:43:GLN:HG3	2.00	0.61
1:B:139:TYR:O	1:B:140:PRO:C	2.39	0.60
3:A:318:ILE:HD12	3:A:342:SER:O	2.02	0.59
2:C:98:SER:O	2:C:109:ASP:HA	2.03	0.59
3:A:343:GLY:H	3:A:378:THR:HB	1.68	0.59
1:B:30:THR:HG21	1:B:90:TRP:CE3	2.38	0.59
3:A:459:THR:H	3:A:462:GLN:NE2	2.00	0.59
1:B:37:GLN:HE22	2:C:39:GLN:HE22	1.51	0.58
3:D:482:CYS:HA	3:D:491:CYS:SG	2.43	0.58
3:D:487:SER:O	3:D:489:GLU:N	2.36	0.58
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.39	0.58
3:A:451:ILE:HD12	3:A:453:TRP:CZ2	2.39	0.58
2:C:29:PHE:HB2	2:C:77:ASN:HD22	1.69	0.58
3:D:380:PHE:HB2	3:D:413:SER:HA	1.87	0.57
3:A:401:ILE:HD11	3:A:403:ARG:CZ	2.35	0.57
1:B:34:TRP:CD2	1:B:72:PHE:HB2	2.39	0.57
3:A:486:CYS:HA	3:A:499:CYS:SG	2.45	0.57
2:H:171:VAL:HB	2:H:190:VAL:HG22	1.86	0.56
1:B:6:GLN:NE2	1:B:101:THR:OG1	2.39	0.56
1:B:37:GLN:O	1:B:83:ALA:HB1	2.06	0.56
2:C:6:GLN:HE22	2:C:96:CYS:N	2.03	0.56
1:L:11:LEU:HD23	1:L:103:VAL:HG22	1.88	0.56
2:C:6:GLN:NE2	2:C:96:CYS:H	2.03	0.55
2:H:208:HIS:ND1	2:H:211:SER:HB3	2.20	0.55
1:L:89:GLN:NE2	1:L:96:THR:HB	2.22	0.55
1:L:165:GLN:HG3	1:L:172:TYR:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:162:TRP:CZ3	2:C:204:CYS:HB3	2.42	0.55
3:A:459:THR:HG23	3:A:461:GLY:H	1.73	0.54
1:L:93:HIS:HA	3:D:459:THR:HG21	1.89	0.53
1:L:113:SER:HB2	1:L:136:ASN:HB3	1.90	0.53
3:D:418:SER:HA	3:D:441:GLY:O	2.09	0.53
1:L:189:LYS:HA	1:L:210:ARG:O	2.07	0.53
1:B:30:THR:CG2	1:B:90:TRP:CE3	2.91	0.53
1:L:117:PHE:CD2	2:H:132:LEU:HB3	2.43	0.53
1:B:30:THR:HG22	1:B:90:TRP:O	2.10	0.52
1:B:65:GLY:HA3	1:B:70:TYR:CD2	2.44	0.52
2:H:91:THR:HG23	2:H:118:THR:HA	1.90	0.52
2:C:32:HIS:HD2	2:C:100:ASP:CB	2.23	0.52
2:C:28:THR:O	2:C:31:SER:HB2	2.09	0.52
1:L:146:GLN:O	1:L:193:CYS:HA	2.09	0.52
3:A:459:THR:HG23	3:A:461:GLY:N	2.24	0.52
2:C:32:HIS:HD2	2:C:100:ASP:HB3	1.75	0.52
2:C:204:CYS:O	2:C:216:ASP:HB3	2.10	0.52
3:A:325:LEU:HD13	4:A:3281:NAG:H83	1.91	0.51
1:B:82:ILE:O	1:B:103:VAL:O	2.27	0.51
1:B:30:THR:HG22	1:B:91:SER:CA	2.33	0.51
2:H:11:VAL:HB	2:H:155:PRO:HG3	1.92	0.51
3:A:483:HIS:CD2	3:A:485:LEU:H	2.28	0.51
2:C:6:GLN:HE21	2:C:112:GLY:HA3	1.76	0.51
2:C:208:HIS:CE1	2:C:210:PRO:HG2	2.46	0.51
2:H:29:PHE:C	2:H:31:SER:H	2.14	0.51
1:B:112:PRO:HD3	1:B:197:HIS:CD2	2.46	0.50
1:L:154:GLN:HB3	1:L:157:ASN:HD21	1.76	0.50
2:C:205:ASN:HA	2:C:216:ASP:HB3	1.93	0.50
2:C:99:ARG:HG2	2:C:109:ASP:HB2	1.94	0.50
2:H:151:LYS:HE3	2:H:179:GLN:NE2	2.27	0.50
1:B:138:PHE:O	1:B:139:TYR:O	2.30	0.49
1:B:49:ASP:O	1:B:50:THR:CB	2.60	0.49
1:L:95:PHE:HB2	2:H:47:TRP:CD2	2.47	0.49
1:B:138:PHE:O	1:B:138:PHE:CD1	2.65	0.49
2:H:16:ALA:O	2:H:86:LEU:HB2	2.13	0.49
1:B:139:TYR:HD2	1:B:140:PRO:HD3	1.60	0.49
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.47	0.49
3:D:386:TRP:CG	3:D:387:PRO:HD2	2.48	0.49
3:A:380:PHE:CB	3:A:413:SER:HA	2.36	0.49
1:B:106:LYS:HA	1:B:139:TYR:OH	2.13	0.48
1:L:93:HIS:HD1	3:D:459:THR:HG23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3281:NAG:O4	4:A:3282:NAG:C2	2.61	0.48
2:C:50:GLU:HG3	2:C:59:ASN:HB2	1.96	0.48
3:D:403:ARG:HA	3:D:433:SER:HB2	1.95	0.48
1:L:89:GLN:HE22	1:L:96:THR:HB	1.79	0.48
3:A:482:CYS:HG	3:A:491:CYS:HB2	1.78	0.48
3:A:492:TRP:H	3:A:498:ASP:HB3	1.78	0.48
1:B:197:HIS:CD2	1:B:199:GLY:H	2.31	0.48
3:A:482:CYS:CB	3:A:491:CYS:HG	2.25	0.48
2:H:40:ALA:O	2:H:43:GLN:HB2	2.13	0.47
1:L:107:ARG:NH1	1:L:110:ALA:HB2	2.29	0.47
2:C:91:THR:HG23	2:C:118:THR:HA	1.96	0.47
4:A:3281:NAG:C4	4:A:3282:NAG:C1	2.93	0.47
1:B:65:GLY:HA3	1:B:70:TYR:HD2	1.79	0.47
1:L:37:GLN:HE22	2:H:39:GLN:NE2	2.07	0.47
1:B:79:PRO:HA	1:B:105:ILE:HD13	1.97	0.47
2:C:47:TRP:HZ2	2:C:50:GLU:HG2	1.80	0.47
3:A:463:LYS:HE2	2:C:101:TYR:CE1	2.50	0.47
1:L:137:ASN:HA	1:L:172:TYR:O	2.15	0.47
1:L:48:TYR:O	1:L:52:ASN:HB2	2.15	0.47
3:A:400:GLU:HA	3:A:428:SER:O	2.15	0.46
2:C:6:GLN:HG2	2:C:22:CYS:HB2	1.98	0.46
3:A:454:LYS:NZ	2:C:100:ASP:OD1	2.47	0.46
3:D:415:ALA:HA	3:D:438:ILE:CG2	2.46	0.46
3:A:367:GLU:O	3:A:370:ILE:HG13	2.16	0.46
3:A:482:CYS:HG	3:A:491:CYS:CB	2.28	0.46
2:C:209:LYS:N	2:C:210:PRO:HD2	2.30	0.46
1:L:105:ILE:O	1:L:165:GLN:NE2	2.37	0.46
1:L:109:VAL:HG13	1:L:140:PRO:HD3	1.98	0.46
1:B:37:GLN:NE2	2:C:39:GLN:HE22	2.13	0.46
2:H:209:LYS:N	2:H:210:PRO:CD	2.79	0.46
2:H:84:SER:O	2:H:85:SER:C	2.54	0.46
3:D:311:LYS:H	3:D:339:THR:HB	1.80	0.45
1:B:95:PHE:HD1	2:C:47:TRP:CE2	2.34	0.45
2:H:192:VAL:HG11	2:H:202:TYR:CZ	2.52	0.45
1:L:185:TYR:CE1	1:L:191:TYR:CE2	3.05	0.45
1:L:77:LEU:HD21	1:L:105:ILE:HG12	1.99	0.45
3:D:412:PHE:CE2	3:D:438:ILE:HB	2.52	0.45
2:C:11:VAL:HB	2:C:155:PRO:HG3	1.99	0.45
1:L:29:VAL:HB	1:L:89:GLN:HG3	1.98	0.45
1:B:45:LEU:HD23	1:B:54:ALA:HB2	1.99	0.45
2:C:51:PHE:O	2:C:53:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:378:THR:HG23	3:A:405:ARG:HH11	1.81	0.44
1:B:107:ARG:HH21	1:B:110:ALA:HB2	1.82	0.44
3:A:459:THR:HB	1:B:93:HIS:CE1	2.52	0.44
2:H:55:ASN:OD1	2:H:57:ARG:HB2	2.17	0.44
3:D:363:LEU:O	3:D:365:PRO:HD3	2.17	0.44
2:H:39:GLN:C	2:H:92:ALA:HB1	2.38	0.44
1:L:33:TYR:HB2	1:L:88:GLN:HG2	1.99	0.44
2:C:7:SER:HB3	2:C:21:SER:H	1.83	0.44
1:L:120:SER:OG	2:H:130:PHE:HB3	2.17	0.44
1:L:208:PHE:CD1	1:L:208:PHE:N	2.86	0.44
1:L:60:ARG:HD2	1:L:74:ILE:HG22	2.00	0.44
3:A:449:ASN:HB3	2:C:103:TYR:CZ	2.53	0.44
2:H:164:SER:HA	2:H:205:ASN:OD1	2.18	0.44
1:B:169:ASP:OD1	1:B:171:THR:OG1	2.23	0.43
2:H:6:GLN:N	2:H:113:GLN:OE1	2.34	0.43
3:D:344:ASP:OD1	3:D:379:GLY:HA3	2.19	0.43
3:A:482:CYS:SG	3:A:491:CYS:SG	3.10	0.43
1:L:6:GLN:HE21	1:L:98:GLY:HA3	1.82	0.43
1:L:29:VAL:HG13	1:L:70:TYR:OH	2.18	0.43
1:B:85:TYR:O	1:B:100:GLY:HA2	2.18	0.43
2:H:4:LEU:HD23	2:H:24:ALA:HA	2.01	0.43
1:B:4:MET:HE1	1:B:25:ALA:HA	2.01	0.43
3:D:486:CYS:O	3:D:488:PRO:HD3	2.19	0.43
2:H:39:GLN:HE21	2:H:95:TYR:HE1	1.66	0.43
1:L:57:VAL:HA	1:L:58:PRO:HD2	1.85	0.43
1:B:3:GLN:H	1:B:26:SER:HG	1.65	0.43
1:L:79:PRO:O	1:L:82:ILE:HD12	2.19	0.43
1:L:208:PHE:HD1	1:L:208:PHE:N	2.16	0.42
2:H:151:LYS:HE2	2:H:179:GLN:HE22	1.83	0.42
1:B:129:ALA:O	1:B:179:THR:HA	2.19	0.42
3:D:394:HIS:CD2	3:D:394:HIS:H	2.37	0.42
2:H:130:PHE:HA	2:H:131:PRO:HD2	1.83	0.42
1:B:36:GLN:HG3	1:B:85:TYR:CZ	2.55	0.42
1:B:86:TYR:HE2	2:C:44:GLY:HA2	1.84	0.42
2:H:28:THR:O	2:H:31:SER:HB2	2.18	0.42
3:A:442:ASN:HB2	3:A:445:LEU:HB3	2.01	0.42
3:D:440:SER:HA	3:D:467:ILE:O	2.19	0.42
1:L:95:PHE:HD1	2:H:47:TRP:CZ2	2.38	0.42
3:A:459:THR:H	3:A:462:GLN:HE21	1.68	0.41
3:D:431:GLU:OE2	3:D:433:SER:OG	2.37	0.41
3:D:364:ASP:O	3:D:366:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:ARG:HA	2:H:108:PHE:O	2.20	0.41
3:A:380:PHE:CD2	3:A:407:LYS:HA	2.55	0.41
3:D:453:TRP:O	3:D:456:LEU:HB2	2.21	0.41
2:H:33:TRP:CH2	2:H:52:ASN:HB2	2.55	0.41
1:L:107:ARG:HH12	1:L:110:ALA:HB2	1.83	0.41
3:D:404:GLY:O	3:D:407:LYS:HE3	2.21	0.41
3:D:380:PHE:CB	3:D:413:SER:HA	2.50	0.41
1:L:31:TYR:OH	3:D:463:LYS:HE2	2.20	0.41
3:A:481:VAL:HG12	3:A:482:CYS:H	1.86	0.41
2:C:155:PRO:HB2	2:C:156:GLU:H	1.67	0.41
1:L:208:PHE:HD1	1:L:208:PHE:H	1.69	0.41
3:A:341:ILE:HD12	3:A:345:LEU:HD11	2.03	0.41
3:D:451:ILE:HA	3:D:490:GLY:HA3	2.02	0.41
3:A:337:ASN:ND2	4:A:3371:NAG:H2	2.36	0.40
3:A:382:LEU:HD12	3:A:415:ALA:HB3	2.02	0.40
3:A:446:CYS:C	3:A:447:TYR:CD2	2.94	0.40
3:A:455:LYS:O	2:C:55:ASN:ND2	2.53	0.40
3:A:312:VAL:HG22	3:A:340:SER:HB3	2.03	0.40
1:B:79:PRO:HA	1:B:105:ILE:CD1	2.52	0.40
2:H:97:ALA:HA	2:H:110:TYR:O	2.21	0.40
3:A:337:ASN:HD21	4:A:3371:NAG:C2	2.34	0.40
1:B:82:ILE:CD1	1:B:105:ILE:HD12	2.52	0.40
1:B:37:GLN:NE2	1:B:43:PRO:HD3	2.37	0.40
1:B:94:ILE:HG22	2:C:47:TRP:HZ3	1.86	0.40
1:L:107:ARG:HG3	1:L:108:THR:O	2.22	0.40
1:B:139:TYR:CD1	1:B:140:PRO:N	2.88	0.40
1:L:117:PHE:HB2	1:L:132:VAL:HB	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	B	167/212 (79%)	145 (87%)	16 (10%)	6 (4%)	3	23
1	L	209/212 (99%)	189 (90%)	15 (7%)	5 (2%)	6	34
2	C	185/223 (83%)	159 (86%)	21 (11%)	5 (3%)	5	30
2	H	212/223 (95%)	190 (90%)	17 (8%)	5 (2%)	6	34
3	A	189/214 (88%)	153 (81%)	32 (17%)	4 (2%)	7	37
3	D	189/214 (88%)	153 (81%)	29 (15%)	7 (4%)	3	22
All	All	1151/1298 (89%)	989 (86%)	130 (11%)	32 (3%)	5	29

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	50	THR
1	B	122	GLU
1	B	139	TYR
1	B	140	PRO
2	H	30	THR
2	H	85	SER
2	H	163	ASN
3	A	443	LYS
3	A	470	ARG
1	B	50	THR
1	B	82	ILE
1	B	137	ASN
2	C	85	SER
2	C	124	THR
2	C	215	VAL
3	D	472	GLU
3	D	488	PRO
2	H	88	SER
3	A	334	HIS
2	C	41	PRO
3	D	443	LYS
3	D	494	PRO
1	L	137	ASN
1	L	190	VAL
3	A	349	PRO
2	H	62	GLU
1	L	26	SER
1	L	203	PRO
3	D	471	GLY
3	D	496	PRO

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Mol	Chain	Res	Type
3	D	421	ILE
2	C	155	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	B	124/188 (66%)	115 (93%)	9 (7%)	14	46
1	L	158/188 (84%)	146 (92%)	12 (8%)	13	45
2	C	122/190 (64%)	106 (87%)	16 (13%)	4	19
2	H	159/190 (84%)	139 (87%)	20 (13%)	4	21
3	A	142/188 (76%)	125 (88%)	17 (12%)	5	22
3	D	118/188 (63%)	109 (92%)	9 (8%)	13	45
All	All	823/1132 (73%)	740 (90%)	83 (10%)	7	29

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	27	SER
1	L	29	VAL
1	L	44	LYS
1	L	59	SER
1	L	73	THR
1	L	89	GLN
1	L	126	SER
1	L	135	LEU
1	L	177	THR
1	L	179	THR
1	L	208	PHE
2	H	7	SER
2	H	31	SER
2	H	46	GLU
2	H	57	ARG

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Mol	Chain	Res	Type
2	H	69	THR
2	H	74	THR
2	H	78	THR
2	H	88	SER
2	H	100	ASP
2	H	113	GLN
2	H	120	SER
2	H	143	THR
2	H	158	VAL
2	H	181	SER
2	H	186	LEU
2	H	191	THR
2	H	194	SER
2	H	200	GLN
2	H	201	THR
2	H	211	SER
3	A	310	LYS
3	A	313	CYS
3	A	320	GLU
3	A	334	HIS
3	A	397	GLU
3	A	401	ILE
3	A	411	GLN
3	A	422	THR
3	A	447	TYR
3	A	449	ASN
3	A	451	ILE
3	A	459	THR
3	A	464	THR
3	A	465	LYS
3	A	475	CYS
3	A	481	VAL
3	A	497	ARG
1	B	14	SER
1	B	15	VAL
1	B	22	THR
1	B	38	LYS
1	B	68	THR
1	B	73	THR
1	B	91	SER
1	B	92	SER
1	B	163	THR

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Mol	Chain	Res	Type
2	C	2	VAL
2	C	7	SER
2	C	11	VAL
2	C	22	CYS
2	C	28	THR
2	C	43	GLN
2	C	86	LEU
2	C	100	ASP
2	C	109	ASP
2	C	113	GLN
2	C	120	SER
2	C	124	THR
2	C	148	CYS
2	C	187	SER
2	C	191	THR
2	C	212	ASN
3	D	320	GLU
3	D	324	SER
3	D	356	SER
3	D	389	ASN
3	D	401	ILE
3	D	422	THR
3	D	440	SER
3	D	459	THR
3	D	491	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	89	GLN
1	L	137	ASN
1	L	154	GLN
1	L	188	HIS
2	H	32	HIS
2	H	39	GLN
2	H	59	ASN
2	H	163	ASN
2	H	172	HIS
2	H	179	GLN
2	H	200	GLN
3	A	328	ASN

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Mol	Chain	Res	Type
3	A	337	ASN
3	A	389	ASN
3	A	462	GLN
3	A	480	GLN
3	A	483	HIS
1	B	37	GLN
1	B	52	ASN
1	B	197	HIS
2	C	6	GLN
2	C	32	HIS
2	C	43	GLN
2	C	77	ASN
2	C	212	ASN
3	D	337	ASN
3	D	384	GLN
3	D	389	ASN
3	D	394	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	3284	-	11,11,12	0.48	0	15,15,17	1.53	2 (13%)
4	NAG	A	4201	-	14,14,15	0.63	0	17,19,21	1.52	3 (17%)
4	NAG	A	3371	-	14,14,15	0.55	0	17,19,21	1.77	4 (23%)
4	NAG	A	4202	-	14,14,15	0.56	0	17,19,21	1.10	1 (5%)
4	NAG	D	3281	-	14,14,15	0.68	0	17,19,21	1.54	3 (17%)
5	BMA	D	3283	-	11,11,12	0.55	0	15,15,17	1.55	2 (13%)
4	NAG	D	3282	-	14,14,15	0.68	0	17,19,21	1.61	2 (11%)
4	NAG	A	3281	-	14,14,15	0.85	1 (7%)	17,19,21	1.82	3 (17%)
5	BMA	A	3283	-	11,11,12	0.45	0	15,15,17	0.82	0
4	NAG	A	3282	-	14,14,15	0.74	0	17,19,21	1.67	3 (17%)
4	NAG	D	3371	-	14,14,15	0.50	0	17,19,21	1.36	2 (11%)
4	NAG	D	3891	-	14,14,15	0.57	0	17,19,21	0.65	0
4	NAG	A	3891	-	14,14,15	0.60	0	17,19,21	1.12	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	3284	-	-	1/2/19/22	0/1/1/1
4	NAG	A	4201	-	-	4/6/23/26	0/1/1/1
4	NAG	A	3371	-	-	2/6/23/26	0/1/1/1
4	NAG	A	4202	-	-	2/6/23/26	0/1/1/1
4	NAG	D	3281	-	-	1/6/23/26	0/1/1/1
5	BMA	D	3283	-	-	0/2/19/22	0/1/1/1
4	NAG	D	3282	-	-	4/6/23/26	0/1/1/1
4	NAG	A	3281	-	-	2/6/23/26	0/1/1/1
5	BMA	A	3283	-	-	1/2/19/22	0/1/1/1
4	NAG	A	3282	-	-	1/6/23/26	0/1/1/1
4	NAG	D	3371	-	-	3/6/23/26	0/1/1/1
4	NAG	D	3891	-	-	2/6/23/26	0/1/1/1
4	NAG	A	3891	-	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3281	NAG	O5-C1	-2.28	1.40	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3281	NAG	O5-C1-C2	-5.30	102.92	111.29
4	D	3371	NAG	C1-O5-C5	4.48	118.26	112.19
4	A	4201	NAG	C3-C4-C5	4.39	118.08	110.24
4	A	3371	NAG	C3-C4-C5	4.35	117.99	110.24
5	D	3283	BMA	C3-C4-C5	4.17	117.68	110.24
4	A	3282	NAG	O5-C1-C2	-4.07	104.85	111.29
6	A	3284	MAN	C1-O5-C5	3.94	117.53	112.19
6	A	3284	MAN	O5-C1-C2	3.63	116.37	110.77
4	A	3281	NAG	C3-C4-C5	3.61	116.68	110.24
4	A	3282	NAG	C4-C3-C2	-3.61	105.73	111.02
4	D	3282	NAG	C3-C4-C5	3.50	116.49	110.24
4	D	3282	NAG	O5-C1-C2	-3.44	105.85	111.29
4	D	3281	NAG	C3-C4-C5	3.28	116.09	110.24
4	A	3371	NAG	O5-C1-C2	-3.07	106.44	111.29
4	A	4201	NAG	O5-C1-C2	-2.96	106.61	111.29
4	A	3281	NAG	C2-N2-C7	-2.91	118.77	122.90
4	A	3371	NAG	C1-O5-C5	2.76	115.93	112.19
5	D	3283	BMA	O5-C1-C2	-2.67	106.65	110.77
4	D	3371	NAG	O5-C1-C2	2.62	115.42	111.29
4	A	3891	NAG	C3-C4-C5	2.60	114.88	110.24
4	D	3281	NAG	O5-C1-C2	-2.47	107.39	111.29
4	A	3891	NAG	O5-C1-C2	-2.46	107.40	111.29
4	D	3281	NAG	O3-C3-C4	-2.44	104.71	110.35
4	A	3371	NAG	O5-C5-C4	2.39	116.64	110.83
4	A	4202	NAG	O5-C5-C6	2.07	110.45	107.20
4	A	3282	NAG	C2-N2-C7	-2.04	119.99	122.90
4	A	4201	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3371	NAG	C8-C7-N2-C2
4	D	3371	NAG	O7-C7-N2-C2
4	A	3891	NAG	C8-C7-N2-C2
4	A	3891	NAG	O7-C7-N2-C2
4	D	3282	NAG	C8-C7-N2-C2
4	D	3282	NAG	O7-C7-N2-C2
4	D	3891	NAG	C8-C7-N2-C2
4	D	3891	NAG	O7-C7-N2-C2
4	A	3281	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	4201	NAG	O5-C5-C6-O6
4	A	3371	NAG	C4-C5-C6-O6
4	A	3281	NAG	C4-C5-C6-O6
4	D	3282	NAG	O5-C5-C6-O6
4	A	4201	NAG	C4-C5-C6-O6
4	A	4202	NAG	O5-C5-C6-O6
4	A	3371	NAG	O5-C5-C6-O6
4	D	3281	NAG	O5-C5-C6-O6
4	A	4201	NAG	C8-C7-N2-C2
6	A	3284	MAN	O5-C5-C6-O6
4	D	3282	NAG	C4-C5-C6-O6
4	A	4201	NAG	O7-C7-N2-C2
4	D	3371	NAG	C4-C5-C6-O6
4	A	3891	NAG	O5-C5-C6-O6
4	A	3282	NAG	O5-C5-C6-O6
4	A	4202	NAG	C4-C5-C6-O6
5	A	3283	BMA	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	3284	MAN	1	0
4	A	3371	NAG	3	0
4	D	3281	NAG	4	0
4	D	3282	NAG	1	0
4	A	3281	NAG	6	0
5	A	3283	BMA	1	0
4	A	3282	NAG	3	0
4	A	3891	NAG	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	B	175/212 (82%)	0.01	4 (2%) 60 47	27, 40, 96, 100	0
1	L	211/212 (99%)	-0.33	1 (0%) 91 86	25, 42, 73, 83	0
2	C	191/223 (85%)	-0.14	8 (4%) 36 23	34, 51, 81, 83	0
2	H	216/223 (96%)	-0.25	0 100 100	31, 50, 63, 69	0
3	A	191/214 (89%)	-0.33	1 (0%) 91 86	34, 47, 76, 81	0
3	D	191/214 (89%)	-0.30	0 100 100	44, 53, 89, 94	0
All	All	1175/1298 (90%)	-0.23	14 (1%) 79 67	25, 49, 82, 100	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	189	VAL	3.4
2	C	128	SER	2.9
2	C	188	SER	2.9
2	C	127	PRO	2.9
1	B	197	HIS	2.5
3	A	484	ALA	2.4
2	C	164	SER	2.2
1	L	191	TYR	2.2
1	B	196	THR	2.2
2	C	165	GLY	2.2
1	B	130	SER	2.1
2	C	150	VAL	2.0
2	C	187	SER	2.0
1	B	133	CYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	A	3283	11/12	0.70	0.26	108,108,108,109	0
4	NAG	A	4202	14/15	0.72	0.42	102,103,103,103	0
5	BMA	D	3283	11/12	0.74	0.20	111,112,112,112	0
4	NAG	D	3371	14/15	0.74	0.27	104,106,106,107	0
4	NAG	D	3891	14/15	0.78	0.24	96,97,98,98	0
4	NAG	A	3891	14/15	0.80	0.20	99,100,100,100	0
4	NAG	A	3371	14/15	0.83	0.23	82,85,85,86	0
6	MAN	A	3284	11/12	0.86	0.18	91,94,95,95	0
4	NAG	A	4201	14/15	0.89	0.21	76,78,78,78	0
4	NAG	A	3282	14/15	0.93	0.20	52,54,55,57	0
4	NAG	D	3282	14/15	0.93	0.15	67,70,73,74	0
4	NAG	A	3281	14/15	0.96	0.20	31,35,42,42	0
4	NAG	D	3281	14/15	0.97	0.16	33,37,39,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.