WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:35 am GMT

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PDB ID	:	3P11
Title	:	anti-EGFR/HER3 Fab DL11 in complex with domains I-III of the HER3 extracellular region
Authors	:	Eigenbrot, C.; Shia, S.
Deposited on	:	2010-09-29
Resolution	:	3.70 Å(reported)

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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 3.70 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	Percentile Ranks	Value
Rfree		0.324
Clashscore		11
Ramachandran outliers		2.0%
Sidechain outliers		7.3%
RSRZ outliers		4.6%

Worse ——— Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
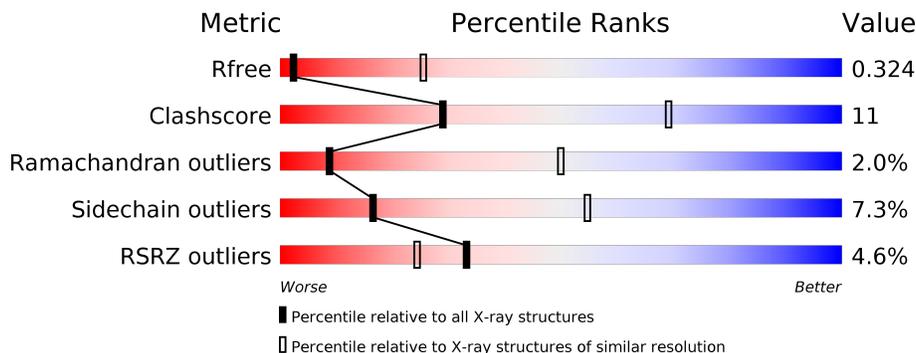
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	H	228	2% — 67% — 26% • •
2	L	214	2% — 73% — 23% • •
3	A	522	7% — 71% — 24% • •

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	623	X	-	-	-
4	NAG	A	627	X	-	-	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7205 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 Fab DL11 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1614	1016	270	322	6			

- Molecule 2 is a protein called Fab DL11 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1624	1018	268	333	5			

- Molecule 3 is a protein called Receptor tyrosine-protein kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	506	Total	C	N	O	S	0	0	0
			3911	2433	705	729	44			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	514	GLY	-	EXPRESSION TAG	UNP P21860
A	515	ASN	-	EXPRESSION TAG	UNP P21860
A	516	SER	-	EXPRESSION TAG	UNP P21860
A	517	HIS	-	EXPRESSION TAG	UNP P21860
A	518	HIS	-	EXPRESSION TAG	UNP P21860
A	519	HIS	-	EXPRESSION TAG	UNP P21860
A	520	HIS	-	EXPRESSION TAG	UNP P21860
A	521	HIS	-	EXPRESSION TAG	UNP P21860
A	522	HIS	-	EXPRESSION TAG	UNP P21860

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
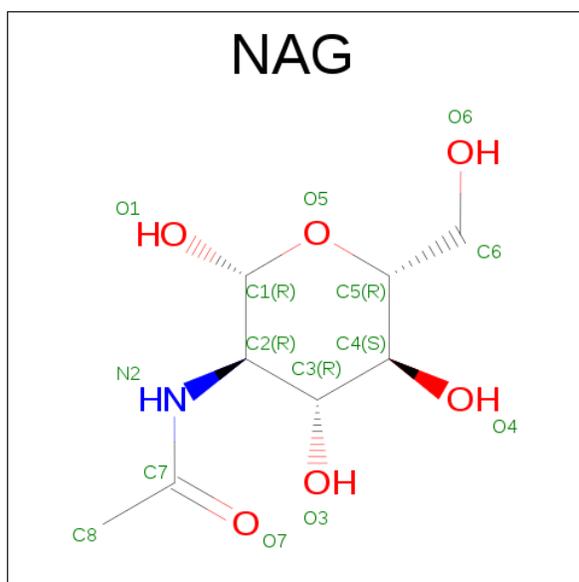
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total 28	C 16	N 2	O 10	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Fab DL11 heavy chain
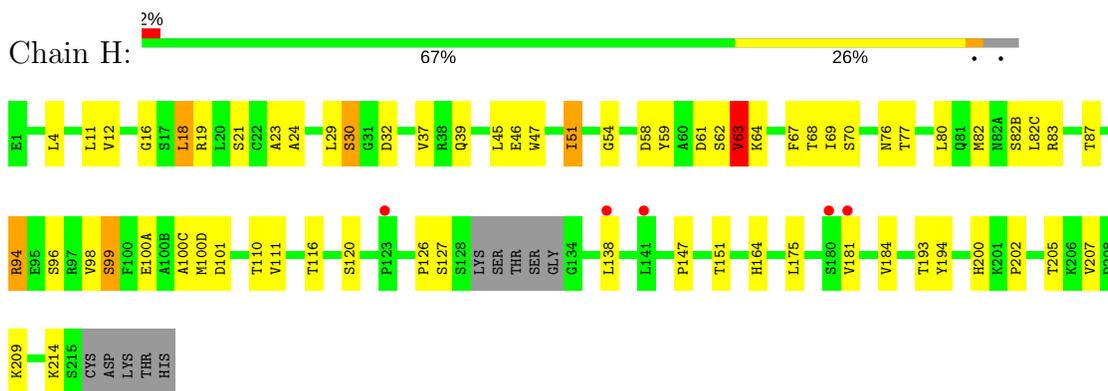
• Molecule 2: Fab DL11 light chain
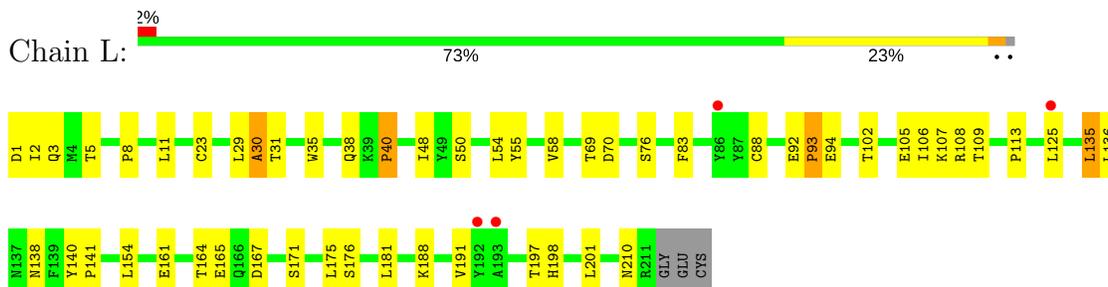
• Molecule 3: Receptor tyrosine-protein kinase erbB-3
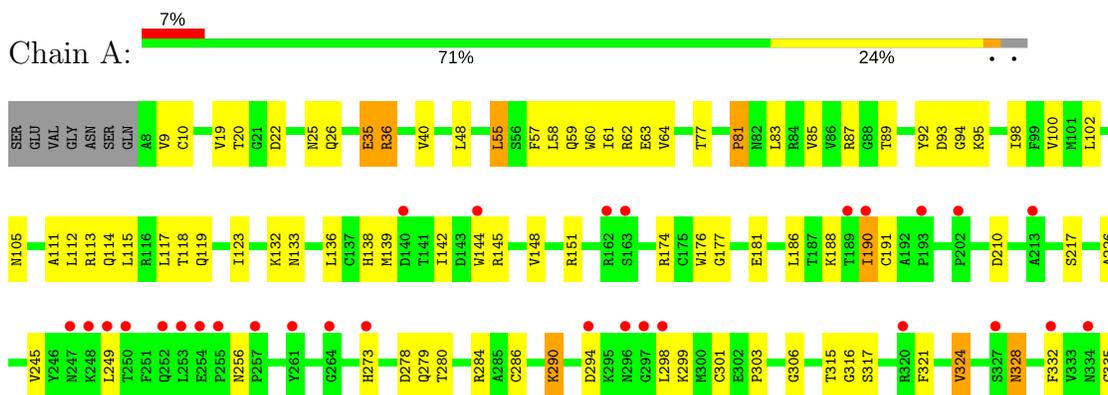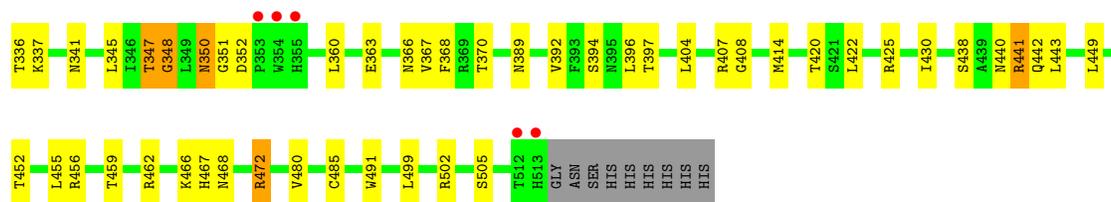
# 4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.39Å 48.40Å 130.38Å 90.00° 127.71° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 45.37 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.70) 99.9 (45.37-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.245 , 0.323 0.240 , 0.324	Depositor DCC
R_{free} test set	574 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	131.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 102.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7205	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	H	0.43	0/1651	0.55	0/2249
2	L	0.40	0/1660	0.57	0/2256
3	A	0.39	0/4002	0.59	1/5432 (0.0%)
All	All	0.40	0/7313	0.58	1/9937 (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
3	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	36	ARG	N-CA-C	-6.79	92.67	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	188	LYS	Peptide
3	A	190	ILE	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	H	1614	0	1570	44	0
2	L	1624	0	1572	36	0
3	A	3911	0	3768	85	0
4	A	28	0	26	3	0
5	A	28	0	25	3	0
All	All	7205	0	6961	154	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 11.

All (154) 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)
3:A:389:ASN:HD21	5:A:624:NAG:C1	1.55	1.20
1:H:30:SER:OG	3:A:407:ARG:HG2	1.60	0.99
3:A:370:THR:HG22	4:A:623:NAG:H82	1.49	0.93
3:A:389:ASN:ND2	5:A:624:NAG:C1	2.33	0.91
2:L:54:LEU:HD22	2:L:58:VAL:HG13	1.58	0.84
1:H:39:GLN:HE22	2:L:38:GLN:HE22	1.28	0.81
2:L:54:LEU:HD22	2:L:58:VAL:CG1	2.10	0.80
3:A:455:LEU:HD11	3:A:462:ARG:NH2	1.98	0.78
2:L:55:TYR:O	2:L:58:VAL:HG12	1.85	0.77
3:A:35:GLU:O	3:A:57:PHE:HB2	1.86	0.75
2:L:30:ALA:HB3	3:A:472:ARG:HD3	1.71	0.73
3:A:466:LYS:HG3	3:A:467:HIS:CD2	2.23	0.73
3:A:77:THR:HG22	3:A:114:GLN:HB2	1.70	0.73
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.69	0.73
3:A:55:LEU:HB3	3:A:58:LEU:HD12	1.71	0.72
3:A:19:VAL:HG12	3:A:20:THR:H	1.54	0.72
1:H:82:MET:HE2	1:H:82(C):LEU:HD21	1.72	0.71
3:A:370:THR:CG2	4:A:623:NAG:H82	2.21	0.69
1:H:30:SER:CB	3:A:407:ARG:HG2	2.22	0.69
1:H:59:TYR:CZ	1:H:69:ILE:HG22	2.28	0.69
3:A:278:ASP:O	3:A:280:THR:N	2.26	0.67
3:A:324:VAL:HA	3:A:328:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:TYR:CE1	1:H:69:ILE:HG22	2.30	0.67
3:A:404:LEU:HD13	3:A:408:GLY:HA2	1.75	0.67
3:A:19:VAL:HG21	3:A:48:LEU:HD12	1.78	0.65
3:A:394:SER:HB2	3:A:425:ARG:HD3	1.80	0.64
2:L:31:THR:HG22	3:A:472:ARG:HH11	1.65	0.62
3:A:407:ARG:O	3:A:407:ARG:HG3	2.00	0.61
3:A:449:LEU:HD21	3:A:491:TRP:CH2	2.35	0.60
2:L:191:VAL:HG22	2:L:210:ASN:HD21	1.66	0.60
3:A:396:LEU:HD12	3:A:397:THR:N	2.17	0.59
1:H:54:GLY:HA3	3:A:414:MET:SD	2.42	0.59
3:A:350:ASN:HD22	3:A:350:ASN:N	2.00	0.59
3:A:298:LEU:HD12	3:A:298:LEU:O	2.03	0.59
1:H:24:ALA:HB3	1:H:76:ASN:ND2	2.18	0.58
3:A:332:PHE:O	3:A:335:CYS:HB2	2.04	0.56
2:L:83:PHE:HZ	2:L:165:GLU:HG3	1.71	0.56
1:H:100(A):GLU:O	3:A:466:LYS:NZ	2.39	0.56
3:A:368:PHE:HB2	3:A:392:VAL:HG13	1.86	0.56
2:L:8:PRO:O	2:L:102:THR:HG23	2.06	0.55
3:A:115:LEU:HG	3:A:136:LEU:HD11	1.89	0.55
1:H:63:VAL:HG22	1:H:67:PHE:CE1	2.41	0.55
1:H:98:VAL:O	1:H:98:VAL:HG23	2.07	0.55
1:H:29:LEU:O	1:H:32:ASP:N	2.38	0.55
3:A:100:VAL:HG12	3:A:133:ASN:ND2	2.22	0.54
3:A:92:TYR:O	3:A:94:GLY:N	2.36	0.54
3:A:336:THR:OG1	3:A:337:LYS:N	2.41	0.54
2:L:92:GLU:HB3	2:L:93:PRO:HD3	1.88	0.54
3:A:139:MET:HA	3:A:142:ILE:HD13	1.88	0.54
3:A:347:THR:O	3:A:351:GLY:N	2.38	0.54
2:L:108:ARG:HG2	2:L:109:THR:N	2.23	0.54
3:A:19:VAL:HG12	3:A:20:THR:N	2.23	0.53
3:A:190:ILE:HG22	3:A:191:CYS:H	1.74	0.53
1:H:30:SER:OG	3:A:407:ARG:CG	2.46	0.53
2:L:54:LEU:HD22	2:L:58:VAL:HG11	1.89	0.52
3:A:40:VAL:HB	3:A:64:VAL:HG22	1.92	0.52
3:A:19:VAL:HG13	3:A:26:GLN:OE1	2.09	0.52
3:A:347:THR:O	3:A:348:GLY:C	2.49	0.52
2:L:11:LEU:C	2:L:11:LEU:HD12	2.30	0.52
3:A:85:VAL:HG21	3:A:226:ALA:HB2	1.92	0.51
1:H:164:HIS:HB2	1:H:181:VAL:HG12	1.91	0.51
2:L:30:ALA:CB	3:A:472:ARG:HD3	2.38	0.51
3:A:81:PRO:O	3:A:119:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:ARG:O	3:A:83:LEU:HD12	2.11	0.51
1:H:87:THR:HG23	1:H:110:THR:HA	1.92	0.51
2:L:2:ILE:HD13	2:L:29:LEU:HD21	1.93	0.51
3:A:430:ILE:O	3:A:455:LEU:HD12	2.11	0.50
1:H:37:VAL:HG13	1:H:46:GLU:O	2.12	0.50
1:H:138:LEU:HD12	1:H:138:LEU:C	2.32	0.50
1:H:18:LEU:HD22	1:H:19:ARG:H	1.76	0.50
1:H:29:LEU:O	1:H:30:SER:C	2.48	0.50
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.94	0.49
3:A:92:TYR:C	3:A:94:GLY:H	2.14	0.49
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.95	0.49
3:A:440:ASN:H	3:A:468:ASN:HD22	1.61	0.49
1:H:23:ALA:HA	1:H:77:THR:HG23	1.94	0.49
2:L:164:THR:HG22	2:L:165:GLU:O	2.13	0.49
2:L:69:THR:HG23	2:L:70:ASP:OD2	2.13	0.48
3:A:111:ALA:O	3:A:113:ARG:HD2	2.13	0.48
3:A:452:THR:HG22	3:A:459:THR:HG21	1.95	0.48
3:A:138:HIS:CD2	3:A:177:GLY:HA2	2.48	0.48
3:A:245:VAL:HG22	3:A:256:ASN:HB2	1.95	0.48
1:H:83:ARG:O	1:H:111:VAL:HG11	2.14	0.48
3:A:22:ASP:HB3	3:A:25:ASN:HB2	1.95	0.48
1:H:200:HIS:HB3	1:H:205:THR:HB	1.95	0.48
2:L:135:LEU:HD22	2:L:136:LEU:N	2.29	0.48
3:A:190:ILE:HG22	3:A:191:CYS:N	2.28	0.47
2:L:92:GLU:CB	2:L:93:PRO:HD3	2.44	0.47
1:H:63:VAL:HG22	1:H:67:PHE:CD1	2.49	0.47
3:A:290:LYS:HG3	3:A:303:PRO:HA	1.97	0.47
3:A:117:LEU:HD12	3:A:176:TRP:CZ3	2.49	0.47
1:H:147:PRO:HD2	1:H:202:PRO:HB3	1.97	0.47
3:A:144:TRP:O	3:A:148:VAL:HG23	2.15	0.46
3:A:422:LEU:HD21	3:A:443:LEU:HD21	1.96	0.46
3:A:98:ILE:HD12	3:A:123:ILE:HD11	1.97	0.46
3:A:278:ASP:HA	3:A:301:CYS:HB2	1.98	0.46
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.96	0.46
2:L:40:PRO:HG3	2:L:165:GLU:HG2	1.97	0.46
3:A:442:GLN:HE22	4:A:627:NAG:H62	1.81	0.46
2:L:161:GLU:HB3	2:L:175:LEU:HD11	1.98	0.46
3:A:9:VAL:HG22	3:A:10:CYS:N	2.31	0.46
2:L:141:PRO:O	2:L:198:HIS:HE1	1.98	0.46
1:H:126:PRO:O	1:H:127:SER:HB2	2.16	0.45
3:A:100:VAL:HG12	3:A:133:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:ARG:HD2	1:H:101:ASP:OD1	2.17	0.45
3:A:63:GLU:HA	3:A:85:VAL:O	2.16	0.45
2:L:29:LEU:O	2:L:31:THR:N	2.49	0.45
3:A:112:LEU:HD21	3:A:115:LEU:HD21	1.99	0.45
1:H:98:VAL:O	1:H:99:SER:CB	2.65	0.45
2:L:191:VAL:HG22	2:L:210:ASN:ND2	2.31	0.45
3:A:441:ARG:HE	3:A:441:ARG:HA	1.82	0.45
2:L:107:LYS:HA	2:L:140:TYR:OH	2.17	0.45
2:L:175:LEU:HD12	2:L:176:SER:H	1.82	0.45
1:H:205:THR:HG22	1:H:207:VAL:HG23	1.99	0.45
1:H:61:ASP:C	1:H:63:VAL:H	2.21	0.45
2:L:11:LEU:O	2:L:11:LEU:HD12	2.16	0.45
2:L:167:ASP:O	2:L:171:SER:HA	2.16	0.44
2:L:2:ILE:CD1	2:L:29:LEU:HD21	2.46	0.44
3:A:363:GLU:O	3:A:366:ASN:ND2	2.51	0.44
3:A:58:LEU:HD23	3:A:61:ILE:HD12	2.00	0.44
1:H:51:ILE:O	1:H:51:ILE:HG23	2.17	0.44
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.99	0.44
3:A:174:ARG:NH1	3:A:186:LEU:HD21	2.33	0.44
3:A:455:LEU:HD11	3:A:462:ARG:HH21	1.79	0.44
1:H:184:VAL:HG11	1:H:194:TYR:CE1	2.52	0.44
2:L:113:PRO:HD2	2:L:201:LEU:CD1	2.48	0.44
3:A:102:LEU:HA	3:A:132:LYS:O	2.18	0.43
3:A:366:ASN:HA	3:A:392:VAL:HG22	1.99	0.43
3:A:87:ARG:HB3	3:A:89:THR:HG23	1.99	0.43
3:A:438:SER:HA	3:A:466:LYS:O	2.19	0.43
2:L:136:LEU:N	2:L:136:LEU:HD12	2.33	0.43
1:H:67:PHE:CE2	1:H:82:MET:HG2	2.53	0.43
3:A:345:LEU:N	3:A:345:LEU:HD23	2.34	0.43
1:H:19:ARG:HA	1:H:80:LEU:O	2.19	0.43
1:H:68:THR:O	1:H:68:THR:HG22	2.18	0.43
3:A:315:THR:CG2	3:A:316:GLY:N	2.82	0.42
3:A:389:ASN:ND2	5:A:624:NAG:O5	2.38	0.42
2:L:92:GLU:HB3	2:L:93:PRO:CD	2.48	0.42
1:H:147:PRO:HD2	1:H:202:PRO:CB	2.49	0.42
2:L:31:THR:HG22	3:A:472:ARG:NH1	2.33	0.42
3:A:420:THR:O	3:A:443:LEU:HD12	2.20	0.41
1:H:96:SER:N	1:H:100(C):ALA:O	2.51	0.41
2:L:106:ILE:CG2	2:L:107:LYS:N	2.83	0.41
3:A:350:ASN:N	3:A:350:ASN:ND2	2.67	0.41
3:A:485:CYS:O	3:A:502:ARG:NE	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:LEU:HD12	1:H:12:VAL:H	1.85	0.41
1:H:59:TYR:OH	1:H:69:ILE:HG22	2.19	0.41
1:H:100(A):GLU:OE2	2:L:50:SER:N	2.54	0.41
3:A:324:VAL:HA	3:A:328:ASN:ND2	2.31	0.41
3:A:117:LEU:O	3:A:118:THR:C	2.59	0.40
3:A:190:ILE:CG2	3:A:191:CYS:H	2.35	0.40
3:A:59:GLN:HG3	3:A:60:TRP:N	2.36	0.40
3:A:139:MET:N	3:A:139:MET:HE2	2.36	0.40
1:H:16:GLY:O	1:H:82(C):LEU:HD12	2.22	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	H	214/228 (94%)	191 (89%)	17 (8%)	6 (3%)	6	43
2	L	209/214 (98%)	190 (91%)	15 (7%)	4 (2%)	9	51
3	A	504/522 (97%)	433 (86%)	62 (12%)	9 (2%)	10	52
All	All	927/964 (96%)	814 (88%)	94 (10%)	19 (2%)	9	50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	35	GLU
3	A	55	LEU
3	A	279	GLN
1	H	99	SER
2	L	30	ALA
2	L	93	PRO
1	H	62	SER
1	H	64	LYS

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Mol	Chain	Res	Type
3	A	328	ASN
3	A	284	ARG
2	L	138	ASN
1	H	30	SER
3	A	81	PRO
2	L	40	PRO
1	H	51	ILE
1	H	63	VAL
3	A	306	GLY
3	A	348	GLY
3	A	367	VAL

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	H	177/186 (95%)	161 (91%)	16 (9%)	11	46
2	L	186/188 (99%)	172 (92%)	14 (8%)	16	53
3	A	441/455 (97%)	412 (93%)	29 (7%)	19	59
All	All	804/829 (97%)	745 (93%)	59 (7%)	16	55

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	H	18	LEU
1	H	21	SER
1	H	58	ASP
1	H	63	VAL
1	H	70	SER
1	H	82(B)	SER
1	H	94	ARG
1	H	100(D)	MET
1	H	116	THR
1	H	120	SER

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Mol	Chain	Res	Type
1	H	151	THR
1	H	175	LEU
1	H	193	THR
1	H	209	LYS
1	H	214	LYS
2	L	1	ASP
2	L	3	GLN
2	L	5	THR
2	L	23	CYS
2	L	76	SER
2	L	88	CYS
2	L	94	GLU
2	L	105	GLU
2	L	125	LEU
2	L	135	LEU
2	L	154	LEU
2	L	181	LEU
2	L	188	LYS
2	L	197	THR
3	A	36	ARG
3	A	93	ASP
3	A	95	LYS
3	A	105	ASN
3	A	145	ARG
3	A	151	ARG
3	A	181	GLU
3	A	210	ASP
3	A	217	SER
3	A	249	LEU
3	A	273	HIS
3	A	286	CYS
3	A	290	LYS
3	A	294	ASP
3	A	299	LYS
3	A	317	SER
3	A	321	PHE
3	A	324	VAL
3	A	341	ASN
3	A	347	THR
3	A	350	ASN
3	A	352	ASP
3	A	360	LEU

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Mol	Chain	Res	Type
3	A	441	ARG
3	A	456	ARG
3	A	472	ARG
3	A	480	VAL
3	A	499	LEU
3	A	505	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	76	ASN
1	H	199	ASN
1	H	200	HIS
2	L	124	GLN
2	L	210	ASN
3	A	256	ASN
3	A	328	ASN
3	A	341	ASN
3	A	350	ASN
3	A	366	ASN
3	A	381	GLN
3	A	389	ASN
3	A	442	GLN
3	A	446	HIS
3	A	467	HIS
3	A	468	ASN
3	A	503	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	NAG	A	624	5	14,14,15	0.78	1 (7%)	15,19,21	1.52	3 (20%)
5	NAG	A	625	5	14,14,15	0.60	0	15,19,21	0.97	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
5	NAG	A	624	5	-	0/6/23/26	0/1/1/1
5	NAG	A	625	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	624	NAG	O5-C1	-2.12	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	624	NAG	O5-C1-C2	-3.98	105.93	111.47
5	A	624	NAG	C1-C2-N2	-2.23	106.67	110.49
5	A	624	NAG	C3-C4-C5	2.55	114.72	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	624	NAG	3	0

5.6 Ligand geometry ⓘ

2 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	#$|Z| > 2$
4	NAG	A	623	3	14,14,15	0.57	0	15,19,21	1.43	3 (20%)
4	NAG	A	627	3	14,14,15	0.55	0	15,19,21	1.40	1 (6%)

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	NAG	A	623	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	627	3	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	627	NAG	O5-C1-C2	-4.58	105.10	111.47
4	A	623	NAG	O7-C7-C8	-2.05	118.32	122.06
4	A	623	NAG	C2-N2-C7	2.28	126.26	122.94
4	A	623	NAG	C1-O5-C5	3.10	116.44	112.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	623	NAG	C1
4	A	627	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	623	NAG	2	0
4	A	627	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	H	218/228 (95%)	0.02	5 (2%)	61	48	116, 146, 179, 194	1 (0%)
2	L	211/214 (98%)	0.19	4 (1%)	67	55	113, 145, 177, 195	0
3	A	506/522 (96%)	0.27	34 (6%)	19	13	119, 164, 234, 318	0
All	All	935/964 (96%)	0.19	43 (4%)	33	24	113, 154, 212, 318	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	255	PRO	7.6
3	A	254	GLU	6.3
3	A	247	ASN	6.0
3	A	253	LEU	5.3
3	A	297	GLY	4.8
3	A	190	ILE	4.8
3	A	296	ASN	4.7
3	A	264	GLY	4.1
3	A	248	LYS	3.9
3	A	252	GLN	3.7
3	A	261	TYR	3.3
2	L	192	TYR	3.1
3	A	294	ASP	3.1
3	A	513	HIS	3.0
3	A	257	PRO	2.9
3	A	250	THR	2.9
3	A	354	TRP	2.8
3	A	144	TRP	2.7
3	A	202	PRO	2.6
3	A	332	PHE	2.6
3	A	320	ARG	2.5
3	A	193	PRO	2.5
3	A	162	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	213	ALA	2.4
2	L	125	LEU	2.4
3	A	163	SER	2.3
3	A	273	HIS	2.3
3	A	249	LEU	2.3
3	A	189	THR	2.3
3	A	334	ASN	2.3
3	A	512	THR	2.2
1	H	138	LEU	2.2
3	A	327	SER	2.2
3	A	298	LEU	2.2
2	L	193	ALA	2.2
1	H	141	LEU	2.1
3	A	353	PRO	2.1
1	H	180	SER	2.1
2	L	86	TYR	2.1
1	H	123	PRO	2.1
3	A	355	HIS	2.0
1	H	181	VAL	2.0
3	A	140	ASP	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	A	624	14/15	0.92	0.29	0.70	145,150,154,156	0
5	NAG	A	625	14/15	0.68	0.35	-	161,166,169,169	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	A	623	14/15	0.49	0.60	-	160,167,172,173	0
4	NAG	A	627	14/15	0.84	0.25	-	151,161,163,168	0

6.5 Other polymers ⓘ

There are no such residues in this entry.