



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:33 am GMT

PDB ID : 4OQT
Title : LINGO-1/Li81 Fab complex
Authors : Pepinsky, R.B.; Arndt, J.W.; Quan, C.; Gao, Y.; Quintero-Monzon, O.; Lee, X.; Mi, S.
Deposited on : 2014-02-10
Resolution : 3.23 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

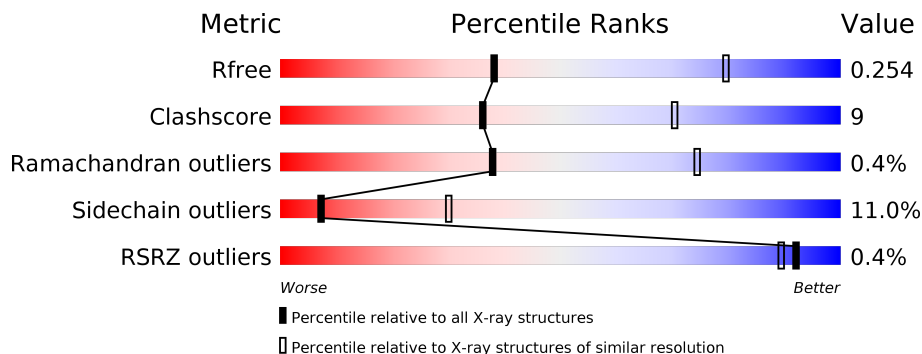
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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}	100719	1247 (3.28-3.20)
Clashscore	112137	1383 (3.28-3.20)
Ramachandran outliers	110173	1358 (3.28-3.20)
Sidechain outliers	110143	1357 (3.28-3.20)
RSRZ outliers	101464	1252 (3.28-3.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	
2	L	215	
3	H	235	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7257 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 Leucine-rich repeat and immunoglobulin-like domain-containing nogo receptor-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3795	2415	679	684	17			

- Molecule 2 is a protein called Light Chain of Li81 Fab, kappa 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1643	1025	278	334	6			

- Molecule 3 is a protein called Heavy Chain of Li81 Fab, VH3-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1618	1019	268	324	7			

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

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

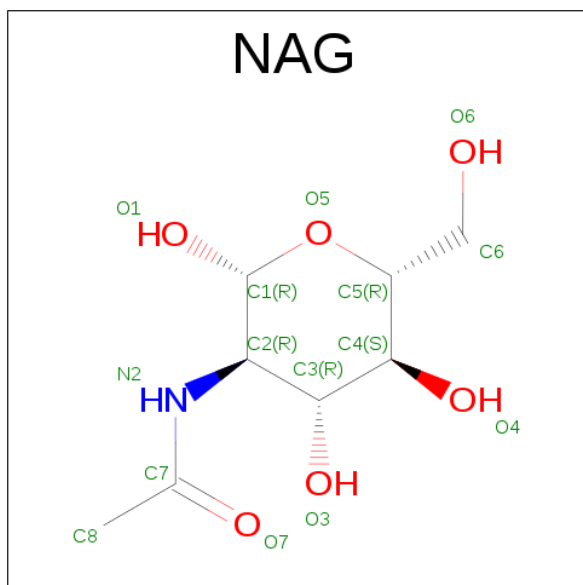
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

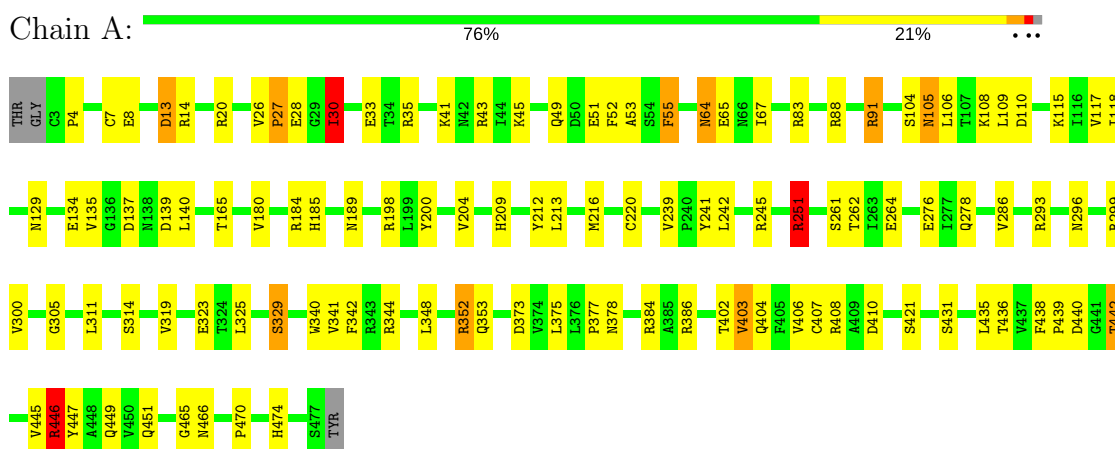


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

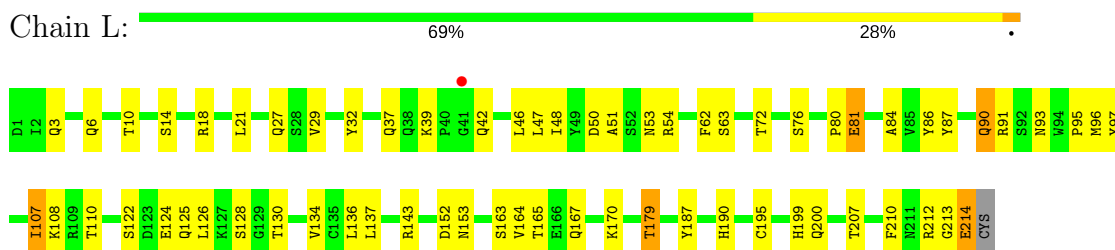
3 Residue-property plots [i](#)

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.

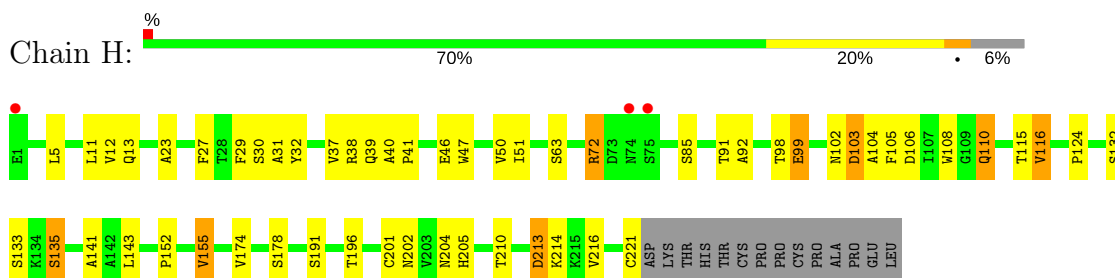
- Molecule 1: Leucine-rich repeat and immunoglobulin-like domain-containing nogo receptor-interacting protein 1



- Molecule 2: Light Chain of Li81 Fab, kappa 3



- Molecule 3: Heavy Chain of Li81 Fab, VH3-23



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.47Å 207.47Å 140.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.23 20.00 – 3.23	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-3.23) 100.0 (20.00-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.192 , 0.256 0.200 , 0.254	Depositor DCC
R_{free} test set	1479 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	99.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7257	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: BMA, 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	A	0.59	0/3877	0.88	5/5272 (0.1%)
2	L	0.60	0/1680	0.78	0/2286
3	H	0.55	0/1656	0.77	0/2259
All	All	0.58	0/7213	0.83	5/9817 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	VAL	C-N-CD	6.41	141.86	128.40
1	A	30	ILE	C-N-CD	5.77	140.52	128.40
1	A	352	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	446	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	251	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3795	0	3799	56	0
2	L	1643	0	1568	43	0
3	H	1618	0	1550	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	117	0	102	6	0
5	A	56	0	50	1	0
6	A	28	0	26	0	0
All	All	7257	0	7095	130	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 9.

All (130) 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:A:30:ILE:CG2	1:A:55:PHE:CE1	2.22	1.22
1:A:30:ILE:HG21	1:A:55:PHE:CE1	1.81	1.15
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.25	1.13
1:A:30:ILE:HG22	1:A:55:PHE:CE1	1.89	1.05
3:H:37:VAL:HG22	3:H:47:TRP:CE3	1.91	1.05
3:H:37:VAL:CG2	3:H:47:TRP:CZ3	2.48	0.96
1:A:30:ILE:CG2	1:A:55:PHE:CD1	2.55	0.90
2:L:37:GLN:CB	2:L:47:LEU:HD11	2.01	0.90
1:A:43:ARG:CZ	1:A:67:ILE:HD11	2.02	0.89
3:H:37:VAL:HG22	3:H:47:TRP:CZ3	2.05	0.88
2:L:47:LEU:O	2:L:48:ILE:HD13	1.79	0.81
2:L:37:GLN:HB2	2:L:47:LEU:CD1	2.11	0.81
1:A:30:ILE:HG21	1:A:55:PHE:CD1	2.17	0.77
1:A:402:THR:HB	1:A:446:ARG:O	1.86	0.76
2:L:134:VAL:HG22	2:L:179:THR:HG23	1.67	0.74
4:A:514:NAG:H4	4:A:515:BMA:O2	1.87	0.74
2:L:91:ARG:NH1	3:H:103:ASP:O	2.20	0.74
2:L:137:LEU:HD12	2:L:137:LEU:N	2.04	0.72
1:A:406:VAL:HG11	1:A:408:ARG:HE	1.54	0.72
1:A:30:ILE:HG22	1:A:55:PHE:CD1	2.20	0.71
1:A:440:ASP:OD1	1:A:442:THR:HG23	1.93	0.68
1:A:198:ARG:NH2	2:L:50:ASP:OD1	2.26	0.67
2:L:213:GLY:O	2:L:214:GLU:HB3	1.94	0.67
1:A:438:PHE:HB3	1:A:439:PRO:HD2	1.76	0.67
1:A:30:ILE:HG22	1:A:55:PHE:HE1	1.51	0.67
1:A:446:ARG:HH21	1:A:446:ARG:HG3	1.60	0.66
2:L:124:GLU:OE1	3:H:214:LYS:NZ	2.28	0.66
2:L:54:ARG:NH1	2:L:62:PHE:O	2.29	0.65
1:A:239:VAL:HB	1:A:241:TYR:CE1	2.32	0.65
1:A:180:VAL:HG22	1:A:204:VAL:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:102:ASN:C	3:H:104:ALA:H	2.02	0.62
1:A:83:ARG:NH2	1:A:105:ASN:OD1	2.33	0.61
1:A:30:ILE:HG21	1:A:55:PHE:CZ	2.35	0.61
1:A:340:TRP:CE2	1:A:341:VAL:HG23	2.39	0.58
1:A:4:PRO:HG2	1:A:7:CYS:SG	2.44	0.57
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.69	0.57
2:L:46:LEU:HD22	3:H:105:PHE:CG	2.39	0.57
1:A:377:PRO:O	1:A:378:ASN:HB2	2.04	0.57
2:L:124:GLU:CD	3:H:214:LYS:NZ	2.58	0.57
3:H:124:PRO:HD2	3:H:210:THR:HG21	1.85	0.56
1:A:403:VAL:HG13	1:A:445:VAL:HB	1.86	0.56
4:A:501:NAG:O4	4:A:502:NAG:H83	2.06	0.55
2:L:91:ARG:HA	2:L:97:TYR:CD1	2.41	0.55
1:A:117:VAL:HA	1:A:139:ASP:O	2.07	0.55
2:L:91:ARG:NH2	3:H:106:ASP:OD1	2.40	0.55
1:A:4:PRO:HB3	1:A:28:GLU:O	2.08	0.54
3:H:11:LEU:HB2	3:H:152:PRO:HG3	1.89	0.54
3:H:132:SER:O	3:H:135:SER:OG	2.20	0.54
2:L:190:HIS:O	2:L:212:ARG:HD3	2.08	0.54
3:H:102:ASN:O	3:H:104:ALA:N	2.41	0.54
2:L:39:LYS:NZ	2:L:81:GLU:O	2.42	0.53
3:H:5:LEU:HD13	3:H:110:GLN:OE1	2.08	0.53
3:H:30:SER:O	3:H:31:ALA:HB3	2.09	0.53
1:A:104:SER:O	1:A:129:ASN:HB2	2.09	0.53
3:H:40:ALA:HB1	3:H:41:PRO:HD2	1.90	0.52
2:L:124:GLU:OE2	3:H:214:LYS:NZ	2.43	0.52
2:L:137:LEU:N	2:L:137:LEU:CD1	2.73	0.52
2:L:29:VAL:HG11	2:L:90:GLN:HG3	1.93	0.51
1:A:216:MET:HB3	1:A:220:CYS:SG	2.51	0.51
2:L:136:LEU:C	2:L:137:LEU:HD12	2.30	0.51
1:A:83:ARG:C	1:A:106:LEU:HD12	2.32	0.51
3:H:116:VAL:O	3:H:116:VAL:HG22	2.11	0.50
1:A:67:ILE:O	1:A:67:ILE:HG22	2.12	0.49
1:A:319:VAL:HG12	1:A:344:ARG:HH12	1.78	0.49
3:H:143:LEU:HB2	3:H:216:VAL:HG11	1.93	0.49
2:L:126:LEU:HD11	2:L:187:TYR:CE2	2.46	0.49
1:A:342:PHE:CE2	1:A:375:LEU:HD11	2.48	0.49
1:A:27:PRO:O	1:A:30:ILE:HD12	2.12	0.49
1:A:305:GLY:HA2	1:A:329:SER:HB3	1.95	0.49
1:A:13:ASP:OD1	1:A:13:ASP:N	2.44	0.48
3:H:155:VAL:HG13	3:H:205:HIS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:47:LEU:CD2	2:L:62:PHE:CD1	2.97	0.48
3:H:5:LEU:HB2	3:H:23:ALA:HB3	1.96	0.48
3:H:32:TYR:CD2	3:H:99:GLU:O	2.67	0.48
2:L:50:ASP:O	2:L:51:ALA:HB3	2.15	0.47
1:A:384:ARG:HG3	1:A:465:GLY:HA3	1.97	0.47
2:L:152:ASP:O	2:L:153:ASN:HB2	2.16	0.46
1:A:276:GLU:HG3	1:A:300:VAL:HB	1.96	0.46
1:A:109:LEU:HD12	1:A:110:ASP:H	1.80	0.46
3:H:32:TYR:HD2	3:H:99:GLU:O	1.97	0.46
2:L:48:ILE:HA	2:L:53:ASN:O	2.16	0.46
1:A:67:ILE:HG23	1:A:91:ARG:CZ	2.46	0.46
3:H:37:VAL:HG21	3:H:47:TRP:CZ3	2.46	0.46
3:H:201:CYS:O	3:H:213:ASP:HA	2.16	0.46
3:H:51:ILE:HD13	3:H:72:ARG:HG2	1.99	0.45
2:L:37:GLN:CB	2:L:47:LEU:CD1	2.84	0.45
2:L:199:HIS:CG	2:L:200:GLN:H	2.34	0.45
1:A:406:VAL:HG12	1:A:407:CYS:N	2.31	0.45
1:A:67:ILE:CG2	1:A:91:ARG:NH1	2.80	0.45
2:L:164:VAL:HG12	2:L:165:THR:O	2.16	0.45
2:L:14:SER:HA	2:L:108:LYS:HB2	1.99	0.45
2:L:84:ALA:HB3	2:L:86:TYR:CE1	2.52	0.45
4:A:514:NAG:C4	4:A:515:BMA:O2	2.61	0.44
1:A:43:ARG:NE	1:A:67:ILE:HD11	2.32	0.44
2:L:210:PHE:CD1	2:L:210:PHE:O	2.70	0.44
1:A:185:HIS:HA	1:A:209:HIS:O	2.17	0.44
1:A:299:ARG:NH1	1:A:299:ARG:HB3	2.31	0.44
1:A:200:TYR:HD2	2:L:32:TYR:CE1	2.35	0.44
1:A:438:PHE:HB3	1:A:439:PRO:CD	2.47	0.44
1:A:278:GLN:HG3	4:A:501:NAG:H82	2.00	0.44
3:H:39:GLN:O	3:H:92:ALA:HB1	2.18	0.43
1:A:14:ARG:HB2	1:A:35:ARG:HB2	2.00	0.43
3:H:108:TRP:N	3:H:108:TRP:CD1	2.87	0.43
2:L:125:GLN:O	2:L:128:SER:HB3	2.17	0.43
1:A:189:ASN:HA	1:A:213:LEU:HA	1.99	0.43
3:H:110:GLN:HE21	3:H:110:GLN:HB3	1.69	0.43
3:H:141:ALA:HB2	3:H:191:SER:HB3	2.01	0.43
3:H:37:VAL:HG12	3:H:38:ARG:N	2.32	0.43
2:L:48:ILE:HG23	2:L:53:ASN:O	2.18	0.43
1:A:323:GLU:O	1:A:348:LEU:HA	2.19	0.43
1:A:212:TYR:CD1	4:A:507:NAG:H81	2.55	0.42
1:A:20:ARG:NH1	1:A:41:LYS:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:214:LYS:HD2	3:H:214:LYS:HA	1.89	0.42
2:L:95:PRO:HB2	3:H:50:VAL:HG21	2.01	0.42
2:L:80:PRO:HA	2:L:107:ILE:HG21	2.02	0.41
3:H:91:THR:HG23	3:H:115:THR:HA	2.00	0.41
4:A:502:NAG:O3	4:A:503:BMA:H2	2.21	0.41
1:A:474:HIS:CE1	5:A:511:NAG:H5	2.55	0.41
1:A:311:LEU:CD2	1:A:325:LEU:HD11	2.49	0.41
2:L:195:CYS:O	2:L:207:THR:HA	2.21	0.41
2:L:214:GLU:HG2	3:H:221:CYS:O	2.21	0.41
1:A:251:ARG:HH11	1:A:251:ARG:HB3	1.85	0.41
1:A:447:TYR:O	1:A:449:GLN:OE1	2.39	0.41
2:L:107:ILE:H	2:L:167:GLN:HE22	1.67	0.41
1:A:51:GLU:HB3	1:A:52:PHE:CD2	2.56	0.40
2:L:21:LEU:N	2:L:21:LEU:HD12	2.36	0.40
1:A:64:ASN:ND2	1:A:64:ASN:H	2.19	0.40
3:H:12:VAL:HG13	3:H:116:VAL:HB	2.03	0.40
3:H:27:PHE:CE2	3:H:29:PHE:HA	2.56	0.40
2:L:199:HIS:CG	2:L:200:GLN:N	2.89	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	A	473/478 (99%)	419 (89%)	52 (11%)	2 (0%)	38	74
2	L	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
3	H	219/235 (93%)	206 (94%)	11 (5%)	2 (1%)	20	61
All	All	904/928 (97%)	821 (91%)	79 (9%)	4 (0%)	38	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
3	H	178	SER
3	H	103	ASP
1	A	470	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	A	423/428 (99%)	375 (89%)	48 (11%)	7	29
2	L	183/187 (98%)	162 (88%)	21 (12%)	6	28
3	H	177/196 (90%)	160 (90%)	17 (10%)	10	36
All	All	783/811 (96%)	697 (89%)	86 (11%)	7	30

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	13	ASP
1	A	27	PRO
1	A	30	ILE
1	A	33	GLU
1	A	45	LYS
1	A	49	GLN
1	A	55	PHE
1	A	64	ASN
1	A	65	GLU
1	A	88	ARG
1	A	91	ARG
1	A	105	ASN
1	A	108	LYS
1	A	115	LYS
1	A	118	ILE
1	A	134	GLU
1	A	135	VAL
1	A	137	ASP

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Mol	Chain	Res	Type
1	A	140	LEU
1	A	165	THR
1	A	184	ARG
1	A	242	LEU
1	A	245	ARG
1	A	251	ARG
1	A	261	SER
1	A	262	THR
1	A	264	GLU
1	A	286	VAL
1	A	293	ARG
1	A	296	ASN
1	A	314	SER
1	A	329	SER
1	A	352	ARG
1	A	353	GLN
1	A	373	ASP
1	A	386	ARG
1	A	403	VAL
1	A	404	GLN
1	A	410	ASP
1	A	421	SER
1	A	431	SER
1	A	435	LEU
1	A	436	THR
1	A	442	THR
1	A	446	ARG
1	A	451	GLN
1	A	466	ASN
2	L	3	GLN
2	L	10	THR
2	L	18	ARG
2	L	27	GLN
2	L	42	GLN
2	L	63	SER
2	L	72	THR
2	L	76	SER
2	L	81	GLU
2	L	90	GLN
2	L	93	ASN
2	L	96	MET
2	L	107	ILE

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Mol	Chain	Res	Type
2	L	110	THR
2	L	122	SER
2	L	130	THR
2	L	143	ARG
2	L	163	SER
2	L	170	LYS
2	L	179	THR
2	L	214	GLU
3	H	13	GLN
3	H	46	GLU
3	H	63	SER
3	H	72	ARG
3	H	85	SER
3	H	98	THR
3	H	99	GLU
3	H	110	GLN
3	H	116	VAL
3	H	133	SER
3	H	135	SER
3	H	155	VAL
3	H	174	VAL
3	H	196	THR
3	H	202	ASN
3	H	204	ASN
3	H	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	349	ASN
1	A	394	GLN
2	L	6	GLN
2	L	139	ASN
2	L	167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

13 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	$\# Z > 2$
4	NAG	A	501	1,4	14,14,15	0.74	0	15,19,21	2.12	4 (26%)
4	NAG	A	502	4	14,14,15	0.78	0	15,19,21	1.17	0
4	BMA	A	503	4	11,11,12	0.56	0	13,15,17	1.99	4 (30%)
5	NAG	A	504	1,5	14,14,15	0.67	0	15,19,21	1.25	1 (6%)
5	NAG	A	505	5	14,14,15	0.73	0	15,19,21	1.75	3 (20%)
4	NAG	A	507	1,4	14,14,15	0.69	0	15,19,21	1.99	5 (33%)
4	NAG	A	508	4	14,14,15	0.92	0	15,19,21	2.62	8 (53%)
4	BMA	A	509	4	11,11,12	0.64	0	13,15,17	2.12	4 (30%)
5	NAG	A	511	1,5	14,14,15	0.50	0	15,19,21	1.76	3 (20%)
5	NAG	A	512	5	14,14,15	0.48	0	15,19,21	2.96	4 (26%)
4	NAG	A	513	1,4	14,14,15	0.65	0	15,19,21	1.78	4 (26%)
4	NAG	A	514	4	14,14,15	0.67	0	15,19,21	2.70	7 (46%)
4	BMA	A	515	4	11,11,12	0.59	0	13,15,17	1.11	1 (7%)

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	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	4	-	0/6/23/26	0/1/1/1
4	BMA	A	503	4	-	0/2/19/22	0/1/1/1
5	NAG	A	504	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	505	5	-	0/6/23/26	0/1/1/1
4	NAG	A	507	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	508	4	-	0/6/23/26	0/1/1/1
4	BMA	A	509	4	-	0/2/19/22	0/1/1/1
5	NAG	A	511	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	512	5	-	0/6/23/26	0/1/1/1
4	NAG	A	513	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	514	4	-	0/6/23/26	0/1/1/1
4	BMA	A	515	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	514	NAG	O5-C1-C2	-5.37	104.00	111.47
4	A	503	BMA	O5-C1-C2	-4.94	103.06	110.79
4	A	507	NAG	C1-C2-N2	-4.45	102.88	110.49
4	A	508	NAG	O5-C1-C2	-4.26	105.55	111.47
5	A	512	NAG	C1-C2-N2	-3.74	104.09	110.49
4	A	514	NAG	O4-C4-C3	-3.45	102.85	110.36
4	A	513	NAG	O5-C1-C2	-3.45	106.67	111.47
4	A	501	NAG	O7-C7-C8	-3.15	116.31	122.06
5	A	511	NAG	C1-C2-N2	-3.09	105.20	110.49
5	A	504	NAG	C1-C2-N2	-3.01	105.35	110.49
4	A	508	NAG	O7-C7-C8	-2.83	116.91	122.06
4	A	508	NAG	O4-C4-C3	-2.68	104.52	110.36
4	A	507	NAG	C8-C7-N2	-2.67	111.29	116.11
4	A	514	NAG	O3-C3-C2	-2.56	103.90	109.39
4	A	503	BMA	O2-C2-C3	-2.47	105.32	110.17
4	A	508	NAG	O7-C7-N2	-2.35	117.39	121.92
4	A	503	BMA	C1-C2-C3	-2.32	106.71	109.65
4	A	509	BMA	O2-C2-C3	-2.16	105.93	110.17
4	A	513	NAG	O3-C3-C2	-2.14	104.80	109.39
4	A	514	NAG	O7-C7-C8	-2.11	118.22	122.06
4	A	513	NAG	O4-C4-C3	-2.09	105.80	110.36
4	A	507	NAG	O5-C1-C2	-2.05	108.63	111.47
4	A	508	NAG	O3-C3-C2	-2.03	105.05	109.39
5	A	505	NAG	C4-C3-C2	2.13	114.14	111.02
5	A	511	NAG	O4-C4-C5	2.30	115.08	109.28
4	A	501	NAG	O7-C7-N2	2.30	126.35	121.92
4	A	501	NAG	C1-C2-N2	2.42	114.62	110.49
4	A	515	BMA	C2-C3-C4	2.49	115.22	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	BMA	C1-O5-C5	2.52	115.64	112.17
4	A	507	NAG	O7-C7-N2	2.63	126.98	121.92
5	A	512	NAG	C8-C7-N2	2.86	121.26	116.11
5	A	505	NAG	C1-O5-C5	2.98	116.27	112.17
4	A	507	NAG	C1-O5-C5	3.07	116.39	112.17
4	A	508	NAG	C1-O5-C5	3.10	116.44	112.17
4	A	509	BMA	O5-C1-C2	3.33	116.00	110.79
4	A	514	NAG	C8-C7-N2	3.44	122.31	116.11
4	A	514	NAG	C1-O5-C5	3.54	117.05	112.17
5	A	512	NAG	C4-C3-C2	3.59	116.27	111.02
4	A	513	NAG	C1-C2-N2	3.70	116.80	110.49
4	A	509	BMA	C1-C2-C3	4.11	114.86	109.65
4	A	508	NAG	C4-C3-C2	4.11	117.04	111.02
4	A	509	BMA	C1-O5-C5	4.41	118.25	112.17
4	A	514	NAG	C4-C3-C2	4.68	117.87	111.02
5	A	505	NAG	C3-C4-C5	4.68	118.46	110.22
5	A	511	NAG	C1-O5-C5	4.68	118.62	112.17
4	A	508	NAG	C8-C7-N2	5.31	125.70	116.11
4	A	501	NAG	C1-O5-C5	6.13	120.61	112.17
5	A	512	NAG	C1-O5-C5	8.64	124.07	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	2	0
4	A	502	NAG	2	0
4	A	503	BMA	1	0
4	A	507	NAG	1	0
5	A	511	NAG	1	0
4	A	514	NAG	2	0
4	A	515	BMA	2	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	$\# Z > 2$
6	NAG	A	506	1	14,14,15	0.73	0	15,19,21	2.48	4 (26%)
6	NAG	A	510	1	14,14,15	1.01	1 (7%)	15,19,21	2.52	5 (33%)

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	NAG	A	506	1	-	0/6/23/26	0/1/1/1
6	NAG	A	510	1	-	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)
6	A	510	NAG	C1-C2	2.83	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	506	NAG	O7-C7-C8	-3.38	115.90	122.06
6	A	510	NAG	O7-C7-C8	-2.98	116.64	122.06
6	A	510	NAG	C4-C3-C2	-2.96	106.69	111.02
6	A	510	NAG	C6-C5-C4	-2.95	106.10	113.00
6	A	506	NAG	C1-O5-C5	3.72	117.29	112.17
6	A	506	NAG	C2-N2-C7	4.64	129.71	122.94
6	A	510	NAG	C1-O5-C5	5.18	119.30	112.17
6	A	510	NAG	O4-C4-C3	5.51	122.34	110.36
6	A	506	NAG	C1-C2-N2	6.08	120.87	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/478 (99%)	-0.55	0 100 100	66, 88, 132, 164	0
2	L	214/215 (99%)	-0.42	1 (0%) 90 87	68, 93, 123, 138	0
3	H	221/235 (94%)	-0.30	3 (1%) 75 65	59, 103, 130, 152	0
All	All	910/928 (98%)	-0.45	4 (0%) 92 89	59, 93, 128, 164	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	74	ASN	2.7
3	H	1	GLU	2.3
2	L	41	GLY	2.1
3	H	75	SER	2.1

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](#)

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	511	14/15	0.93	0.15	-0.52	90,98,105,106	0
4	NAG	A	501	14/15	0.95	0.14	-0.79	73,77,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	504	14/15	0.97	0.14	-0.90	75,84,90,95	0
4	NAG	A	513	14/15	0.98	0.11	-1.21	65,73,78,78	0
4	NAG	A	507	14/15	0.97	0.12	-1.87	78,89,98,106	0
5	NAG	A	512	14/15	0.93	0.29	-	97,129,142,157	0
4	NAG	A	502	14/15	0.92	0.34	-	74,98,107,127	0
4	BMA	A	515	11/12	0.81	0.30	-	95,114,126,135	0
4	NAG	A	508	14/15	0.93	0.19	-	76,84,100,127	0
4	NAG	A	514	14/15	0.94	0.28	-	70,81,90,101	0
5	NAG	A	505	14/15	0.83	0.31	-	114,131,145,155	0
4	BMA	A	503	11/12	0.67	0.30	-	98,121,155,176	0
4	BMA	A	509	11/12	0.91	0.22	-	100,112,125,131	0

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. 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(\AA^2)	Q<0.9
6	NAG	A	510	14/15	0.82	0.31	-	113,142,163,171	0
6	NAG	A	506	14/15	0.76	0.48	-	114,138,156,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.