



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:28 AM UTC

PDB ID : 6CU0 / pdb_00006cu0
Title : Crystal structure of 4-1BBL/4-1BB (C121S) complex in P21 space group
Authors : Aruna, B.; Zajonc, D.M.; Doukov, T.
Deposited on : 2018-03-23
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 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

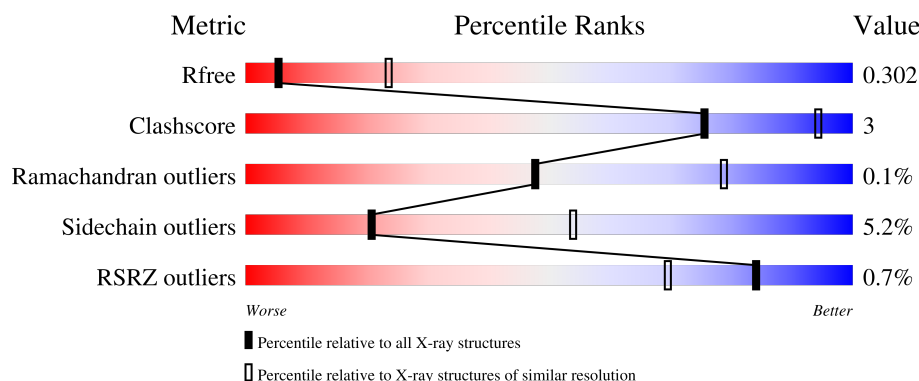
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	165	 79% 12% .. 8%
1	B	165	 80% 8% • 11%
1	C	165	 79% 8% • 11%
1	D	165	 78% 11% • 11%
1	E	165	 78% 8% • 13%

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Mol	Chain	Length	Quality of chain
1	F	165	% 77%14%8%
2	G	138	88%7%5%
2	H	138	% 90%6%
2	I	138	89%6%5%
2	J	138	% 87%7%7%
2	K	138	% 91%
2	L	138	2% 86%7%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11476 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O		0	0	0
			1072	692	185	195				
1	B	147	Total	C	N	O	S	0	0	0
			1033	666	179	187	1			
1	C	147	Total	C	N	O		0	0	0
			999	644	169	186				
1	D	147	Total	C	N	O	S	0	0	0
			1023	656	177	189	1			
1	E	144	Total	C	N	O	S	0	0	0
			987	631	171	184	1			
1	F	151	Total	C	N	O	S	0	0	0
			1046	672	182	191	1			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	131	Total	C	N	O	S	0	0	0
			880	517	158	184	21			
2	H	132	Total	C	N	O	S	0	0	0
			899	527	161	190	21			
2	J	129	Total	C	N	O	S	0	0	0
			865	507	154	183	21			
2	K	132	Total	C	N	O	S	0	0	0
			868	507	158	182	21			
2	L	129	Total	C	N	O	S	0	0	0
			863	506	153	184	20			
2	I	131	Total	C	N	O	S	0	0	0
			869	511	151	186	21			

There are 6 discrepancies between the modelled and reference sequences:

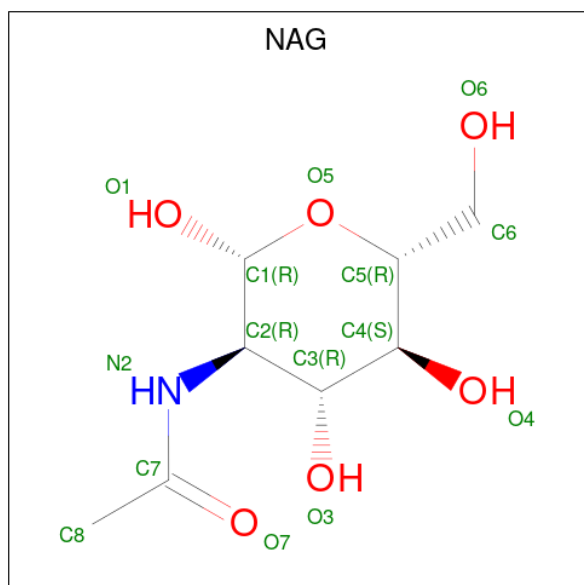
Chain	Residue	Modelled	Actual	Comment	Reference
G	121	SER	CYS	engineered mutation	UNP Q07011

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Chain	Residue	Modelled	Actual	Comment	Reference
H	121	SER	CYS	engineered mutation	UNP Q07011
J	121	SER	CYS	engineered mutation	UNP Q07011
K	121	SER	CYS	engineered mutation	UNP Q07011
L	121	SER	CYS	engineered mutation	UNP Q07011
I	121	SER	CYS	engineered mutation	UNP Q07011

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	2	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

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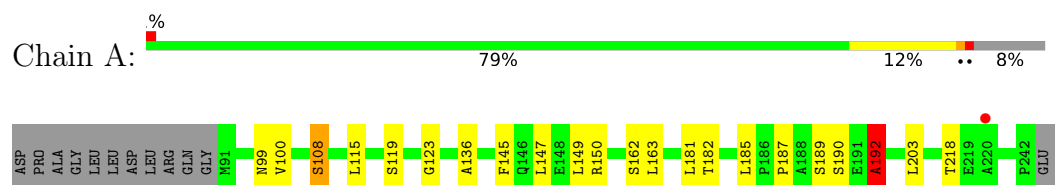
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	O 1	0	0
4	G	7	Total 7	O 7	0	0
4	H	3	Total 3	O 3	0	0
4	J	5	Total 5	O 5	0	0
4	K	13	Total 13	O 13	0	0
4	L	2	Total 2	O 2	0	0
4	I	4	Total 4	O 4	0	0

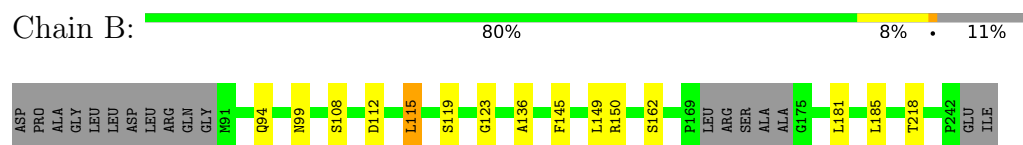
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

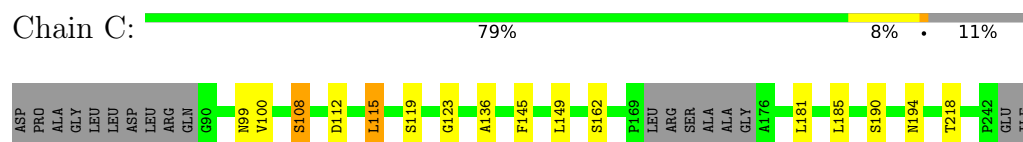
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



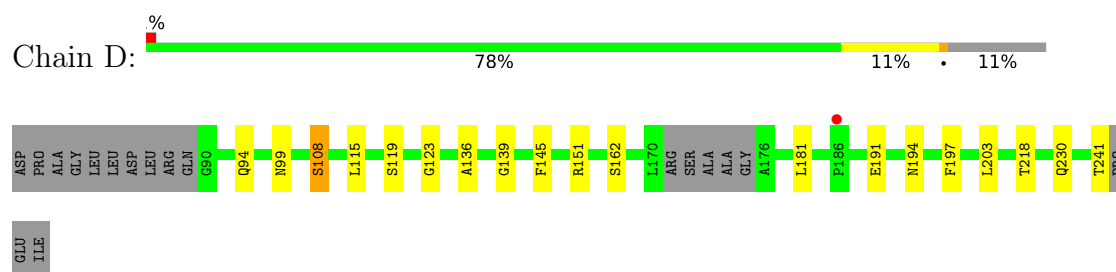
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



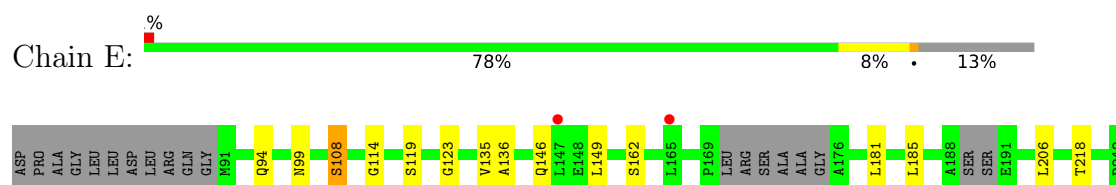
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9



GLU
TLE

- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain F:  77% 14% 8%

ASP PRO ALA GLY LEU LEU ASP ARG GLN G90 A97 Q98 N99 S108 S119 G123 A136 F145 L149 G155 S162 Q168 P169 L170 A173 ALA GLY A176 L181 L185 A188 E191 A192 R193 N194 R202 L203 H215 T218 P242

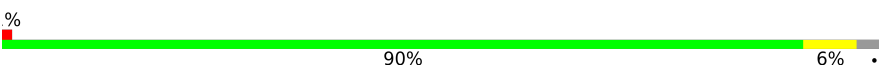
GLU
TLE

- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain G:  88% 7% 5%

SER LEU LEU D26 S52 F53 I64 Q67 K76 N83 S100 C139 V146 LEU VAL N149 E153 C158 GLY PRO

- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain H:  90% 6% 4%

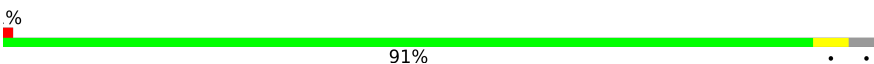
SER LEU LEU D26 F53 G57 GLY Q59 R60 T61 Q67 N83 C99 S121 E153 C158 GLY PRO

- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain J:  87% 7% 7%

SER LEU LEU GLN ASP P27 F53 C65 R66 Q67 N83 C99 C139 D142 GLY LYS SER V146 N149 C150 E153 C158 GLY PRO

- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain K:  91% 7% 2%

SER LEU LEU Q25 F53 Q67 N83 S100 K107 GLN G109 T124 F125 N126 M136 D155 VAL V157 C158 GLY PRO

- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain L:  86% 7% 7%

SER LEU LEU GLN ASP PRO CYS S29 N30 C31 A33 F53 Q67 N83 M101 V146 N149 G150 T151 K152 E153 V156 V157 C158 GLY PRO

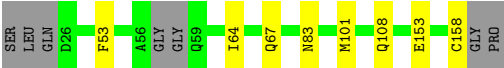
- Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain I:

89%

6%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.96Å 114.75Å 126.04Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-3.20) 94.6 (50.00-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.247 , 0.296 0.258 , 0.302	Depositor DCC
R_{free} test set	1668 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	126.3	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 164.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11476	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: 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	0.67	0/1095	0.91	2/1501 (0.1%)
1	B	0.59	0/1054	0.78	0/1443
1	C	0.59	0/1017	0.78	1/1398 (0.1%)
1	D	0.64	0/1043	0.77	0/1428
1	E	0.63	0/1006	0.80	0/1377
1	F	0.57	0/1068	0.81	1/1464 (0.1%)
2	G	0.68	0/894	0.80	0/1214
2	H	0.66	0/913	0.82	0/1239
2	I	0.69	0/883	0.82	0/1204
2	J	0.61	0/879	0.83	0/1193
2	K	0.62	0/880	0.78	0/1195
2	L	0.71	0/875	0.85	1/1187 (0.1%)
All	All	0.64	0/11607	0.81	5/15843 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	PRO	CA-C-O	-12.78	111.85	121.31
1	F	192	ALA	N-CA-C	6.43	120.29	111.54
1	C	190	SER	N-CA-C	-6.18	104.54	111.28
1	A	192	ALA	N-CA-C	5.10	121.67	110.80
2	L	149	ASN	N-CA-C	5.06	116.80	111.28

There are no chirality outliers.

There are no planarity outliers.

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	A	1072	0	1029	11	0
1	B	1033	0	990	7	0
1	C	999	0	943	6	0
1	D	1023	0	956	10	0
1	E	987	0	909	7	0
1	F	1046	0	986	12	0
2	G	880	0	701	5	0
2	H	899	0	717	3	0
2	I	869	0	669	4	0
2	J	865	0	675	3	0
2	K	868	0	677	5	0
2	L	863	0	676	5	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
4	A	5	0	0	1	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	1	0
4	H	3	0	0	1	0
4	I	4	0	0	0	0
4	J	5	0	0	1	0
4	K	13	0	0	3	0
4	L	2	0	0	0	0
All	All	11476	0	9954	64	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 3.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:149:ASN:OD1	2:J:150:GLY:N	1.94	1.00
2:L:146:VAL:HA	2:L:158:CYS:SG	2.01	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:O	1:A:192:ALA:HB2	1.87	0.73
1:D:139:GLY:HA3	1:D:241:THR:HG21	1.69	0.73
1:D:151:ARG:HE	1:D:194:ASN:HD22	1.37	0.73
2:H:99:CYS:SG	4:H:601:HOH:O	2.48	0.72
1:E:114:GLY:O	2:H:61:THR:HB	1.90	0.71
2:J:99:CYS:SG	4:J:204:HOH:O	2.51	0.69
1:F:191:GLU:N	1:F:191:GLU:OE1	2.24	0.68
2:K:124:THR:HA	4:K:201:HOH:O	1.96	0.64
1:D:115:LEU:HD22	2:I:64:ILE:HD13	1.78	0.64
1:C:112:ASP:HB3	1:C:115:LEU:HD22	1.79	0.63
1:B:112:ASP:HB3	1:B:115:LEU:HD22	1.79	0.63
1:A:115:LEU:HD22	2:G:64:ILE:HD13	1.81	0.61
2:K:136:TRP:CD1	4:K:201:HOH:O	2.53	0.61
1:F:170:LEU:HD12	1:F:173:ALA:C	2.28	0.59
2:K:136:TRP:N	4:K:201:HOH:O	2.36	0.58
1:F:168:GLN:HA	1:F:169:PRO:C	2.29	0.57
1:F:193:ARG:O	1:F:194:ASN:OD1	2.25	0.55
1:F:170:LEU:O	1:F:170:LEU:HD23	2.07	0.55
1:C:194:ASN:ND2	2:L:101:MET:HE1	2.22	0.54
1:A:190:SER:HA	4:A:304:HOH:O	2.07	0.54
1:C:149:LEU:HD13	1:C:185:LEU:HD21	1.90	0.54
1:B:149:LEU:HD13	1:B:185:LEU:HD21	1.88	0.53
2:L:146:VAL:CA	2:L:158:CYS:SG	2.89	0.53
1:E:149:LEU:HD13	1:E:185:LEU:HD21	1.90	0.52
1:A:149:LEU:HD13	1:A:185:LEU:HD21	1.91	0.52
1:B:150:ARG:NH2	2:K:100:SER:O	2.43	0.52
1:F:149:LEU:HD13	1:F:185:LEU:HD21	1.90	0.52
1:E:146:GLN:HE22	1:F:202:ARG:HD2	1.74	0.51
1:F:170:LEU:CD1	1:F:173:ALA:C	2.85	0.49
1:A:150:ARG:NH2	2:G:100:SER:O	2.47	0.48
1:E:94:GLN:HB2	1:F:203:LEU:HD12	1.95	0.47
2:L:150:GLY:O	2:L:151:THR:HB	2.14	0.47
1:B:94:GLN:HB2	1:D:203:LEU:HD12	1.99	0.45
1:D:230:GLN:HE22	2:I:67:GLN:H	1.65	0.45
1:A:182:THR:HB	1:D:197:PHE:CE2	2.53	0.44
1:B:112:ASP:HB3	1:B:115:LEU:CD2	2.47	0.44
1:E:123:GLY:HA3	1:E:136:ALA:HB3	2.00	0.43
1:C:112:ASP:HB3	1:C:115:LEU:CD2	2.46	0.43
1:A:123:GLY:HA3	1:A:136:ALA:HB3	2.01	0.43
1:D:194:ASN:OD1	2:I:101:MET:HE1	2.19	0.43
1:F:155:GLY:HA2	1:F:188:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	2:G:52:SER:HB3	2.01	0.43
1:F:99:ASN:HD21	1:F:108:SER:N	2.17	0.43
1:C:99:ASN:HD21	1:C:108:SER:N	2.17	0.43
1:B:99:ASN:HD21	1:B:108:SER:N	2.17	0.42
1:A:99:ASN:HD21	1:A:108:SER:N	2.17	0.42
1:C:123:GLY:HA3	1:C:136:ALA:HB3	2.02	0.42
1:F:123:GLY:HA3	1:F:136:ALA:HB3	2.02	0.42
2:L:53:PHE:CZ	2:L:83:ASN:HB2	2.55	0.42
1:D:99:ASN:HD21	1:D:108:SER:N	2.17	0.42
2:I:53:PHE:CZ	2:I:83:ASN:HB2	2.54	0.42
1:B:123:GLY:HA3	1:B:136:ALA:HB3	2.01	0.42
2:H:53:PHE:CZ	2:H:83:ASN:HB2	2.55	0.41
2:G:53:PHE:CZ	2:G:83:ASN:HB2	2.55	0.41
2:K:53:PHE:CZ	2:K:83:ASN:HB2	2.55	0.41
1:E:99:ASN:HD21	1:E:108:SER:N	2.17	0.41
2:J:53:PHE:CZ	2:J:83:ASN:HB2	2.56	0.41
2:G:76:LYS:NZ	4:G:601:HOH:O	2.53	0.41
1:A:147:LEU:HD22	1:A:163:LEU:HG	2.03	0.40
1:A:203:LEU:HD12	1:D:94:GLN:HB2	2.04	0.40
1:D:123:GLY:HA3	1:D:136:ALA:HB3	2.01	0.40
1:E:135:VAL:HG21	1:E:206:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/165 (91%)	142 (95%)	7 (5%)	1 (1%)	18	52
1	B	143/165 (87%)	139 (97%)	4 (3%)	0	100	100
1	C	143/165 (87%)	136 (95%)	7 (5%)	0	100	100
1	D	143/165 (87%)	136 (95%)	6 (4%)	1 (1%)	18	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	138/165 (84%)	133 (96%)	5 (4%)	0	100	100
1	F	147/165 (89%)	143 (97%)	4 (3%)	0	100	100
2	G	127/138 (92%)	116 (91%)	11 (9%)	0	100	100
2	H	128/138 (93%)	117 (91%)	11 (9%)	0	100	100
2	I	127/138 (92%)	116 (91%)	11 (9%)	0	100	100
2	J	125/138 (91%)	116 (93%)	9 (7%)	0	100	100
2	K	126/138 (91%)	115 (91%)	11 (9%)	0	100	100
2	L	125/138 (91%)	114 (91%)	11 (9%)	0	100	100
All	All	1622/1818 (89%)	1523 (94%)	97 (6%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	GLU
1	A	192	ALA

5.3.2 Protein sidechains [i](#)

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	98/125 (78%)	91 (93%)	7 (7%)	13	44
1	B	94/125 (75%)	88 (94%)	6 (6%)	16	48
1	C	89/125 (71%)	81 (91%)	8 (9%)	9	34
1	D	91/125 (73%)	85 (93%)	6 (7%)	15	47
1	E	86/125 (69%)	81 (94%)	5 (6%)	18	51
1	F	94/125 (75%)	87 (93%)	7 (7%)	13	43
2	G	91/120 (76%)	87 (96%)	4 (4%)	25	59
2	H	94/120 (78%)	90 (96%)	4 (4%)	26	59
2	I	89/120 (74%)	86 (97%)	3 (3%)	32	64
2	J	88/120 (73%)	84 (96%)	4 (4%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	87/120 (72%)	86 (99%)	1 (1%)	65	79
2	L	87/120 (72%)	85 (98%)	2 (2%)	44	70
All	All	1088/1470 (74%)	1031 (95%)	57 (5%)	21	54

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	VAL
1	A	108	SER
1	A	119	SER
1	A	145	PHE
1	A	162	SER
1	A	181	LEU
1	A	218	THR
1	B	115	LEU
1	B	119	SER
1	B	145	PHE
1	B	162	SER
1	B	181	LEU
1	B	218	THR
1	C	100	VAL
1	C	108	SER
1	C	115	LEU
1	C	119	SER
1	C	145	PHE
1	C	162	SER
1	C	181	LEU
1	C	218	THR
1	D	108	SER
1	D	119	SER
1	D	145	PHE
1	D	162	SER
1	D	181	LEU
1	D	218	THR
1	E	108	SER
1	E	119	SER
1	E	162	SER
1	E	181	LEU
1	E	218	THR
1	F	108	SER
1	F	119	SER

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Mol	Chain	Res	Type
1	F	145	PHE
1	F	162	SER
1	F	181	LEU
1	F	215	HIS
1	F	218	THR
2	G	67	GLN
2	G	139	CYS
2	G	153	GLU
2	G	158	CYS
2	H	67	GLN
2	H	121	SER
2	H	153	GLU
2	H	158	CYS
2	J	67	GLN
2	J	139	CYS
2	J	153	GLU
2	J	158	CYS
2	K	67	GLN
2	L	67	GLN
2	L	153	GLU
2	I	108	GLN
2	I	153	GLU
2	I	158	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	99	ASN
1	A	146	GLN
1	A	200	GLN
1	A	210	GLN
1	B	99	ASN
1	B	200	GLN
1	B	205	HIS
1	B	210	GLN
1	C	98	GLN
1	C	99	ASN
1	C	146	GLN
1	C	200	GLN
1	C	210	GLN
1	D	98	GLN

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Mol	Chain	Res	Type
1	D	99	ASN
1	D	194	ASN
1	D	200	GLN
1	D	210	GLN
1	D	230	GLN
1	E	98	GLN
1	E	99	ASN
1	E	146	GLN
1	E	200	GLN
1	E	210	GLN
1	F	99	ASN
1	F	200	GLN
1	F	205	HIS
1	F	210	GLN
2	G	59	GLN
2	G	138	ASN
2	H	138	ASN
2	J	138	ASN
2	K	59	GLN
2	K	138	ASN
2	L	59	GLN
2	L	138	ASN
2	I	67	GLN
2	I	138	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 ⓘ

There are no oligosaccharides in this entry.

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	$\# Z > 2$
3	NAG	H	501	2	14,14,15	0.82	1 (7%)	17,19,21	1.30	3 (17%)
3	NAG	G	500	2	14,14,15	0.39	0	17,19,21	1.44	3 (17%)

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
3	NAG	H	501	2	-	0/6/23/26	0/1/1/1
3	NAG	G	500	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	501	NAG	C1-C2	2.66	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	500	NAG	C1-O5-C5	3.33	116.65	112.19
3	H	501	NAG	C1-C2-N2	3.07	115.27	110.43
3	H	501	NAG	C1-O5-C5	2.76	115.89	112.19
3	G	500	NAG	C4-C3-C2	-2.45	107.42	111.02
3	G	500	NAG	O5-C1-C2	-2.39	107.59	111.29
3	H	501	NAG	C2-N2-C7	2.28	125.95	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	500	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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(Å ²)	Q<0.9
1	A	152/165 (92%)	-0.46	1 (0%) 84 69	88, 121, 179, 235	0
1	B	147/165 (89%)	-0.38	0 100 100	98, 144, 191, 224	0
1	C	147/165 (89%)	-0.37	0 100 100	109, 139, 179, 189	0
1	D	147/165 (89%)	-0.38	1 (0%) 84 69	100, 132, 175, 211	0
1	E	144/165 (87%)	-0.26	2 (1%) 73 54	107, 143, 180, 205	0
1	F	151/165 (91%)	-0.43	1 (0%) 84 69	112, 156, 206, 244	0
2	G	131/138 (94%)	-0.32	0 100 100	104, 149, 199, 226	0
2	H	132/138 (95%)	-0.34	1 (0%) 82 67	30, 156, 238, 249	0
2	I	131/138 (94%)	-0.38	0 100 100	120, 156, 268, 313	0
2	J	129/138 (93%)	-0.22	2 (1%) 70 51	30, 198, 234, 249	0
2	K	132/138 (95%)	-0.15	1 (0%) 82 67	183, 231, 275, 298	0
2	L	129/138 (93%)	-0.19	3 (2%) 61 41	30, 167, 224, 235	0
All	All	1672/1818 (91%)	-0.33	12 (0%) 84 69	30, 154, 237, 313	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	149	ASN	4.6
1	E	165	LEU	4.5
2	H	59	GLN	4.4
1	E	147	LEU	3.6
2	J	146	VAL	3.1
2	L	150	GLY	2.5
2	L	156	VAL	2.5
2	K	126	ASN	2.3
1	D	186	PRO	2.2
1	F	97	ALA	2.2
1	A	220	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	65	CYS	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
3	NAG	H	501	14/15	0.81	0.07	186,195,202,204	0
3	NAG	G	500	14/15	0.90	0.08	190,198,201,201	0

6.5 Other polymers [i](#)

There are no such residues in this entry.