



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:22 AM UTC

PDB ID : 7NEF / pdb_00007nef
Title : Fucosylated linear peptide Fln65 bound to the fucose binding lectin LecB PA-IIL from *Pseudomonas aeruginosa* at 1.5 Angstrom resolution
Authors : Personne, H.; Baeriswyl, S.; Stocker, A.; Reymond, J.-L.
Deposited on : 2021-02-03
Resolution : 1.51 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

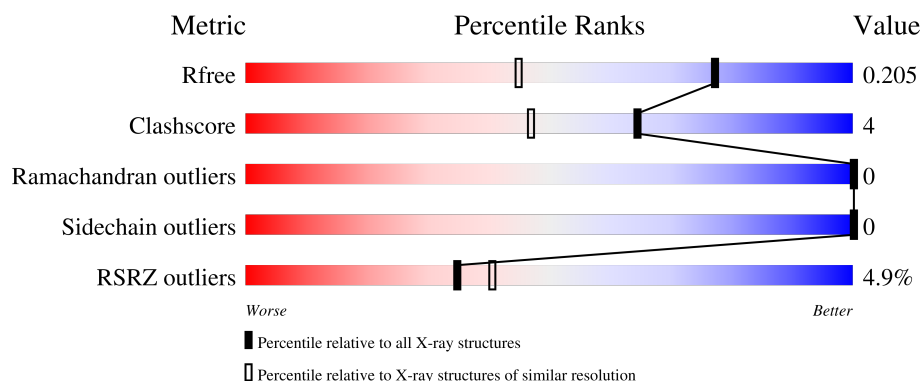
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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.



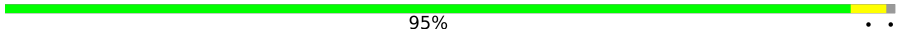
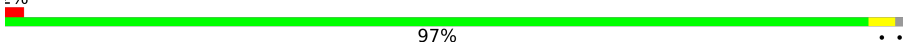
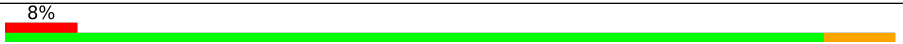
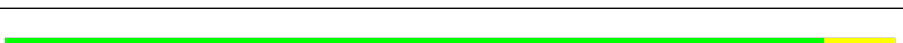
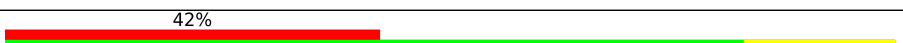
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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 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	115	95%
1	B	115	94%
1	C	115	93%
1	D	115	97%
1	E	115	94%

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Mol	Chain	Length	Quality of chain
1	F	115	
1	G	115	
1	H	115	
2	I	12	
2	J	12	
2	K	12	
2	L	12	
2	M	12	
2	N	12	
2	O	12	
2	P	12	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16227 atoms, of which 7412 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 Fucose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	H	N	O	0	0	0
			1603	504	785	140	174			
1	B	114	Total	C	H	N	O	0	0	0
			1611	506	789	140	176			
1	C	114	Total	C	H	N	O	0	0	0
			1592	503	779	138	172			
1	D	114	Total	C	H	N	O	0	0	0
			1596	503	781	139	173			
1	E	114	Total	C	H	N	O	0	0	0
			1603	504	785	140	174			
1	F	114	Total	C	H	N	O	0	0	0
			1611	506	789	140	176			
1	G	114	Total	C	H	N	O	0	0	0
			1592	503	779	138	172			
1	H	114	Total	C	H	N	O	0	0	0
			1596	503	781	139	173			

- Molecule 2 is a protein called Flh65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			
2	J	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			
2	K	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			
2	L	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			
2	M	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			
2	N	12	Total	C	H	N	O	0	0	1
			223	66	130	16	11			

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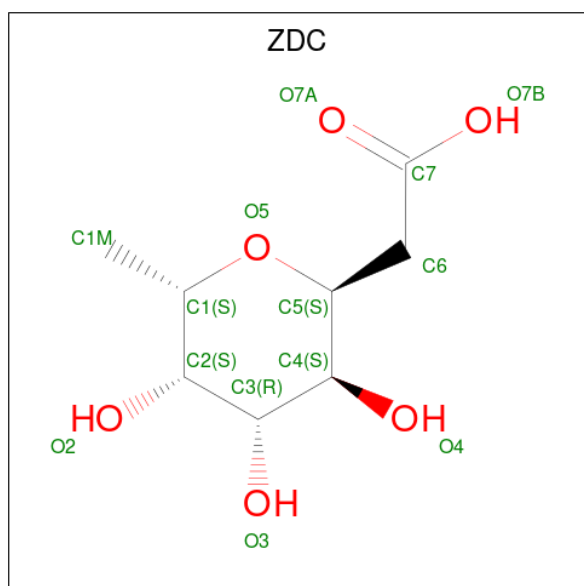
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	12	Total 223	C 66	H 130	N 16	O 11	0	0	1
2	P	12	Total 223	C 66	H 130	N 16	O 11	0	0	1

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	B	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0
3	D	2	Total 2	Ca 2	0	0
3	E	2	Total 2	Ca 2	0	0
3	F	2	Total 2	Ca 2	0	0
3	G	2	Total 2	Ca 2	0	0
3	H	2	Total 2	Ca 2	0	0

- Molecule 4 is 3,7-anhydro-2,8-dideoxy-L-glycero-D-gluco-octonic acid (CCD ID: ZDC) (formula: C₈H₁₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total C H O 26 8 13 5	0	0
4	J	1	Total C H O 26 8 13 5	0	0
4	K	1	Total C H O 26 8 13 5	0	0
4	L	1	Total C H O 26 8 13 5	0	0
4	M	1	Total C H O 26 8 13 5	0	0
4	N	1	Total C H O 26 8 13 5	0	0
4	O	1	Total C H O 26 8 13 5	0	0
4	P	1	Total C H O 26 8 13 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	170	Total O 170 170	0	0
5	B	170	Total O 170 170	0	0
5	C	173	Total O 173 173	0	0
5	D	155	Total O 155 155	0	0
5	E	154	Total O 154 154	0	0
5	F	172	Total O 172 172	0	0
5	G	157	Total O 157 157	0	0
5	H	165	Total O 165 165	0	0
5	I	12	Total O 12 12	0	0
5	J	4	Total O 4 4	0	0
5	K	15	Total O 15 15	0	0
5	L	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	19	Total 19	O 19	0	0
5	N	11	Total 11	O 11	0	0
5	O	23	Total 23	O 23	0	0
5	P	6	Total 6	O 6	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.

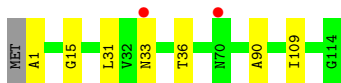
- Molecule 1: Fucose-binding lectin



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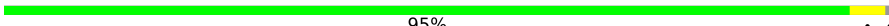
- Molecule 1: Fucose-binding lectin

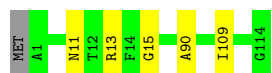


- Molecule 1: Fucose-binding lectin

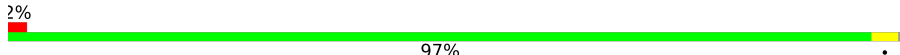


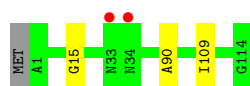
- Molecule 1: Fucose-binding lectin

Chain F:  95% ..

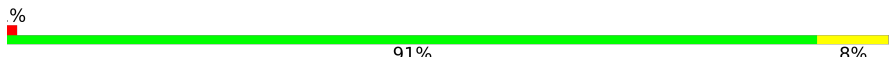


• Molecule 1: Fucose-binding lectin

Chain G:  2% 97% ..



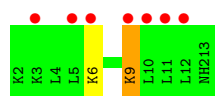
• Molecule 1: Fucose-binding lectin

Chain H:  % 91% 8% .



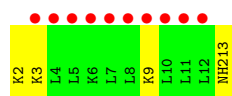
• Molecule 2: Fln65

Chain I:  58% 83% 8% 8%

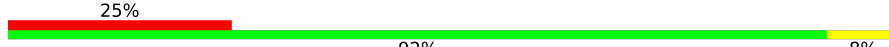


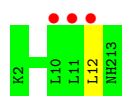
• Molecule 2: Fln65

Chain J:  83% 67% 33%

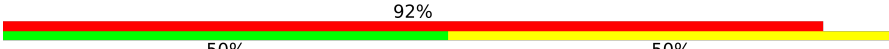


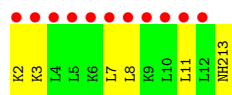
• Molecule 2: Fln65

Chain K:  25% 92% 8%

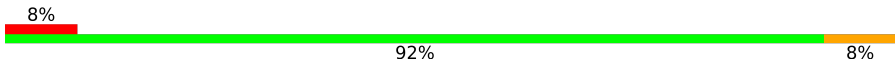


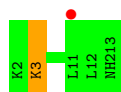
• Molecule 2: Fln65

Chain L:  92% 50% 50%



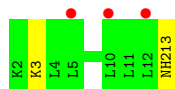
● Molecule 2: Fln65

Chain M:  8% 92% 8%



● Molecule 2: Fln65

Chain N:  25% 83% 17%



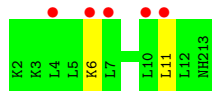
● Molecule 2: Fln65

Chain O:  92% 8%



● Molecule 2: Fln65

Chain P:  42% 83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 64.30Å 118.93Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	48.59 – 1.51 48.59 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.59-1.51) 98.1 (48.59-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.206 0.181 , 0.205	Depositor DCC
R_{free} test set	8641 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.4	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	0.95	EDS
Total number of atoms	16227	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8463e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZDC, CA, NH2

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	0.33	0/828	0.53	0/1135
1	B	0.34	0/832	0.55	0/1140
1	C	0.34	0/823	0.54	0/1128
1	D	0.34	0/825	0.55	0/1131
1	E	0.36	0/828	0.58	0/1135
1	F	0.35	0/832	0.56	0/1140
1	G	0.35	0/823	0.56	0/1128
1	H	0.32	0/825	0.56	0/1131
2	I	0.53	0/91	0.90	1/118 (0.8%)
2	J	0.18	0/91	0.42	0/118
2	K	0.26	0/91	0.34	0/118
2	L	0.48	0/91	0.80	0/118
2	M	0.63	0/91	1.11	2/118 (1.7%)
2	N	0.21	0/91	0.31	0/118
2	O	0.24	0/91	0.37	0/118
2	P	0.20	0/91	0.33	0/118
All	All	0.35	0/7344	0.56	3/10012 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	LYS	CD-CE-NZ	-10.06	79.70	111.90
2	I	9	LYS	CD-CE-NZ	-8.78	83.82	111.90
2	M	3	LYS	CG-CD-CE	-5.70	98.18	111.30

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	818	785	787	5	0
1	B	822	789	791	5	0
1	C	813	779	781	5	0
1	D	815	781	783	2	0
1	E	818	785	787	6	0
1	F	822	789	791	4	0
1	G	813	779	781	2	0
1	H	815	781	783	7	0
2	I	93	130	128	3	0
2	J	93	130	128	3	0
2	K	93	130	128	3	0
2	L	93	130	128	8	0
2	M	93	130	128	1	0
2	N	93	130	128	3	0
2	O	93	130	128	1	0
2	P	93	130	128	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	I	13	13	9	0	0
4	J	13	13	9	0	0
4	K	13	13	9	0	0
4	L	13	13	9	0	0
4	M	13	13	9	0	0
4	N	13	13	9	0	0
4	O	13	13	9	0	0
4	P	13	13	9	0	0
5	A	170	0	0	0	0
5	B	170	0	0	1	0
5	C	173	0	0	3	0
5	D	155	0	0	1	0
5	E	154	0	0	4	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	172	0	0	2	1
5	G	157	0	0	1	2
5	H	165	0	0	2	2
5	I	12	0	0	1	0
5	J	4	0	0	1	0
5	K	15	0	0	3	0
5	L	9	0	0	2	0
5	M	19	0	0	0	0
5	N	11	0	0	2	0
5	O	23	0	0	1	0
5	P	6	0	0	2	0
All	All	8815	7412	7380	57	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (57) 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:81:VAL:HG21	1:B:81:VAL:HG21	1.36	1.07
1:E:33:ASN:ND2	5:E:401:HOH:O	1.96	0.99
2:L:3:LYS:NZ	5:L:201:HOH:O	2.01	0.93
1:H:13:ARG:NH2	5:H:401:HOH:O	2.11	0.83
1:C:33:ASN:OD1	5:C:401:HOH:O	1.95	0.82
2:K:12:LEU:O	5:K:201:HOH:O	1.96	0.82
1:E:33:ASN:OD1	5:E:402:HOH:O	2.03	0.74
5:G:467:HOH:O	1:H:86:GLU:CB	2.38	0.71
2:P:6:LYS:NZ	5:P:1202:HOH:O	2.24	0.69
2:L:8:LEU:O	2:L:11:LEU:HB2	1.94	0.68
2:J:9:LYS:O	2:J:13:NH2:N	2.27	0.67
5:D:403:HOH:O	2:L:3:LYS:HE3	1.96	0.66
5:C:443:HOH:O	1:D:86:GLU:CB	2.43	0.66
2:L:13:NH2:N	5:L:202:HOH:O	2.29	0.65
2:I:9:LYS:O	2:I:9:LYS:HD3	1.98	0.63
1:A:81:VAL:CG2	1:B:81:VAL:HG21	2.24	0.57
2:P:6:LYS:NZ	5:P:1201:HOH:O	1.86	0.56
1:C:1:ALA:N	5:C:402:HOH:O	2.34	0.54
1:F:11:ASN:ND2	5:F:401:HOH:O	2.29	0.54
1:D:90:ALA:HB3	1:D:109:ILE:HB	1.94	0.50
2:J:2:LYS:HG3	5:J:201:HOH:O	2.11	0.49
1:E:90:ALA:HB3	1:E:109:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:9:LYS:HD3	2:I:9:LYS:C	2.38	0.49
2:L:2:LYS:HE3	2:N:13:NH2:N	2.28	0.48
1:B:90:ALA:HB3	1:B:109:ILE:HB	1.96	0.48
2:J:3:LYS:HB3	2:P:11:LEU:HD21	1.95	0.47
1:F:13:ARG:HD3	5:F:519:HOH:O	2.14	0.47
2:L:7:LEU:O	2:L:11:LEU:HG	2.14	0.47
1:F:90:ALA:HB3	1:F:109:ILE:HB	1.96	0.47
1:H:90:ALA:HB3	1:H:109:ILE:HB	1.98	0.46
2:M:3:LYS:HE3	2:M:3:LYS:HA	1.98	0.46
2:I:6:LYS:HD2	5:I:201:HOH:O	2.15	0.46
1:E:29:ASN:ND2	5:E:405:HOH:O	2.46	0.46
2:N:3:LYS:NZ	5:N:201:HOH:O	2.25	0.45
1:A:90:ALA:HB3	1:A:109:ILE:HB	1.98	0.45
1:H:26:GLN:O	1:H:41:SER:HA	2.16	0.44
1:G:90:ALA:HB3	1:G:109:ILE:HB	1.98	0.44
1:F:15:GLY:O	1:F:109:ILE:HA	2.18	0.44
1:B:31:LEU:HD23	1:B:36:THR:HA	1.99	0.43
2:K:12:LEU:HB3	5:K:201:HOH:O	2.18	0.43
1:H:77:VAL:HG12	5:H:470:HOH:O	2.18	0.43
1:C:31:LEU:HD23	1:C:36:THR:HA	1.99	0.43
1:B:15:GLY:O	1:B:109:ILE:HA	2.19	0.43
1:A:83:LEU:HD22	5:B:457:HOH:O	2.19	0.42
1:C:90:ALA:HB3	1:C:109:ILE:HB	2.00	0.42
1:E:33:ASN:N	5:E:401:HOH:O	2.33	0.42
2:N:3:LYS:NZ	5:N:202:HOH:O	2.52	0.42
2:O:3:LYS:HA	5:O:211:HOH:O	2.20	0.41
1:H:31:LEU:HD12	1:H:31:LEU:N	2.36	0.41
1:H:103:ASN:OD1	1:H:103:ASN:C	2.64	0.41
1:A:15:GLY:O	1:A:109:ILE:HA	2.20	0.41
2:L:8:LEU:O	2:L:11:LEU:N	2.54	0.41
1:E:26:GLN:O	1:E:41:SER:HA	2.21	0.41
1:G:15:GLY:O	1:G:109:ILE:HA	2.20	0.41
2:K:12:LEU:C	5:K:201:HOH:O	2.57	0.41
1:C:15:GLY:O	1:C:109:ILE:HA	2.21	0.40
2:L:8:LEU:O	2:L:11:LEU:CB	2.68	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:471:HOH:O	5:H:402:HOH:O[2_644]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:401:HOH:O	5:G:500:HOH:O[2_544]	1.91	0.29
5:G:528:HOH:O	5:H:533:HOH:O[2_544]	1.95	0.25
5:E:500:HOH:O	5:E:508:HOH:O[2_644]	2.18	0.02

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	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	B	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
1	C	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	D	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	E	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	F	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	G	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
1	H	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
2	I	10/12 (83%)	10 (100%)	0	0	100	100
2	J	10/12 (83%)	9 (90%)	1 (10%)	0	100	100
2	K	10/12 (83%)	10 (100%)	0	0	100	100
2	L	10/12 (83%)	7 (70%)	3 (30%)	0	100	100
2	M	10/12 (83%)	10 (100%)	0	0	100	100
2	N	10/12 (83%)	10 (100%)	0	0	100	100
2	O	10/12 (83%)	10 (100%)	0	0	100	100
2	P	10/12 (83%)	10 (100%)	0	0	100	100
All	All	976/1016 (96%)	949 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	91/94 (97%)	91 (100%)	0	100	100
1	B	92/94 (98%)	92 (100%)	0	100	100
1	C	89/94 (95%)	89 (100%)	0	100	100
1	D	90/94 (96%)	90 (100%)	0	100	100
1	E	91/94 (97%)	91 (100%)	0	100	100
1	F	92/94 (98%)	92 (100%)	0	100	100
1	G	89/94 (95%)	89 (100%)	0	100	100
1	H	90/94 (96%)	90 (100%)	0	100	100
2	I	11/11 (100%)	11 (100%)	0	100	100
2	J	11/11 (100%)	11 (100%)	0	100	100
2	K	11/11 (100%)	11 (100%)	0	100	100
2	L	11/11 (100%)	11 (100%)	0	100	100
2	M	11/11 (100%)	11 (100%)	0	100	100
2	N	11/11 (100%)	11 (100%)	0	100	100
2	O	11/11 (100%)	11 (100%)	0	100	100
2	P	11/11 (100%)	11 (100%)	0	100	100
All	All	812/840 (97%)	812 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	29	ASN
1	A	47	ASN
1	A	110	ASN
1	B	21	ASN
1	B	47	ASN

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Mol	Chain	Res	Type
1	B	64	GLN
1	B	110	ASN
1	C	21	ASN
1	C	47	ASN
1	C	80	GLN
1	C	110	ASN
1	D	21	ASN
1	D	47	ASN
1	D	70	ASN
1	D	110	ASN
1	E	21	ASN
1	E	29	ASN
1	E	47	ASN
1	E	66	GLN
1	E	110	ASN
1	F	21	ASN
1	F	47	ASN
1	F	110	ASN
1	G	110	ASN
1	H	21	ASN
1	H	47	ASN
1	H	100	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ZDC	M	101	3	13,13,14	0.96	0	18,18,20	2.27	6 (33%)
4	ZDC	K	101	3	13,13,14	0.84	0	18,18,20	2.30	5 (27%)
4	ZDC	O	101	3	13,13,14	0.89	0	18,18,20	2.04	5 (27%)
4	ZDC	P	101	3	13,13,14	0.83	0	18,18,20	2.40	5 (27%)
4	ZDC	J	101	3	13,13,14	0.78	0	18,18,20	2.40	4 (22%)
4	ZDC	N	101	3	13,13,14	0.89	0	18,18,20	2.40	4 (22%)
4	ZDC	I	101	3	13,13,14	0.80	0	18,18,20	2.31	5 (27%)
4	ZDC	L	101	3	13,13,14	0.87	0	18,18,20	2.18	3 (16%)

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	ZDC	M	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	K	101	3	-	1/3/23/24	0/1/1/1
4	ZDC	O	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	P	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	J	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	N	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	I	101	3	-	2/3/23/24	0/1/1/1
4	ZDC	L	101	3	-	2/3/23/24	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	101	ZDC	C6-C5-C4	6.94	122.72	114.16
4	K	101	ZDC	C6-C5-C4	6.63	122.34	114.16
4	M	101	ZDC	C6-C5-C4	6.59	122.29	114.16
4	N	101	ZDC	C6-C5-C4	6.40	122.06	114.16
4	J	101	ZDC	C6-C5-C4	6.39	122.05	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	101	ZDC	C6-C5-C4	6.13	121.72	114.16
4	O	101	ZDC	C6-C5-C4	5.84	121.36	114.16
4	L	101	ZDC	C6-C5-C4	5.73	121.23	114.16
4	N	101	ZDC	O7A-C7-C6	-4.95	110.97	125.38
4	J	101	ZDC	O7A-C7-C6	-4.82	111.35	125.38
4	K	101	ZDC	O7A-C7-C6	-4.79	111.44	125.38
4	I	101	ZDC	O7A-C7-C6	-4.43	112.49	125.38
4	L	101	ZDC	O7A-C7-C6	-4.40	112.57	125.38
4	M	101	ZDC	O7A-C7-C6	-4.09	113.47	125.38
4	J	101	ZDC	O5-C5-C6	3.81	123.47	109.98
4	P	101	ZDC	O7A-C7-C6	-3.73	114.54	125.38
4	L	101	ZDC	O5-C5-C6	3.70	123.08	109.98
4	O	101	ZDC	O7A-C7-C6	-3.44	115.36	125.38
4	P	101	ZDC	O5-C5-C6	3.37	121.91	109.98
4	P	101	ZDC	C3-C4-C5	-3.22	104.40	110.23
4	O	101	ZDC	O5-C5-C6	3.09	120.93	109.98
4	I	101	ZDC	C3-C4-C5	-3.09	104.63	110.23
4	N	101	ZDC	O5-C5-C6	3.06	120.81	109.98
4	J	101	ZDC	C3-C4-C5	-2.89	104.99	110.23
4	N	101	ZDC	C3-C4-C5	-2.84	105.08	110.23
4	I	101	ZDC	C5-C6-C7	2.84	117.67	112.72
4	O	101	ZDC	O2-C2-C3	-2.70	104.00	110.38
4	K	101	ZDC	C3-C4-C5	-2.57	105.58	110.23
4	M	101	ZDC	C5-C6-C7	2.47	117.03	112.72
4	K	101	ZDC	O5-C5-C6	2.46	118.69	109.98
4	P	101	ZDC	O2-C2-C3	-2.46	104.58	110.38
4	I	101	ZDC	O5-C5-C6	2.45	118.66	109.98
4	M	101	ZDC	C3-C4-C5	-2.43	105.83	110.23
4	M	101	ZDC	O5-C5-C6	2.36	118.33	109.98
4	K	101	ZDC	C5-C6-C7	2.28	116.70	112.72
4	M	101	ZDC	C5-O5-C1	-2.10	107.75	112.71
4	O	101	ZDC	C5-C6-C7	2.04	116.28	112.72

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	101	ZDC	O5-C5-C6-C7
4	M	101	ZDC	O5-C5-C6-C7
4	N	101	ZDC	O5-C5-C6-C7
4	O	101	ZDC	O5-C5-C6-C7
4	P	101	ZDC	O5-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	I	101	ZDC	C5-C6-C7-O7A
4	J	101	ZDC	O5-C5-C6-C7
4	J	101	ZDC	C5-C6-C7-O7A
4	L	101	ZDC	O5-C5-C6-C7
4	L	101	ZDC	C5-C6-C7-O7A
4	M	101	ZDC	C5-C6-C7-O7A
4	N	101	ZDC	C5-C6-C7-O7A
4	O	101	ZDC	C5-C6-C7-O7A
4	P	101	ZDC	C5-C6-C7-O7A
4	K	101	ZDC	C5-C6-C7-O7A

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

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	114/115 (99%)	-0.15	1 (0%) 81 84	13, 16, 26, 53	0
1	B	114/115 (99%)	-0.10	1 (0%) 81 84	12, 16, 26, 44	0
1	C	114/115 (99%)	-0.14	2 (1%) 67 73	12, 15, 26, 33	0
1	D	114/115 (99%)	-0.17	0 100 100	12, 15, 25, 45	0
1	E	114/115 (99%)	-0.18	2 (1%) 67 73	11, 15, 28, 42	0
1	F	114/115 (99%)	-0.15	0 100 100	11, 15, 27, 37	0
1	G	114/115 (99%)	-0.13	2 (1%) 67 73	11, 15, 27, 43	0
1	H	114/115 (99%)	-0.14	1 (0%) 81 84	12, 15, 27, 50	0
2	I	11/12 (91%)	2.24	7 (63%) 0 0	26, 40, 56, 61	0
2	J	11/12 (91%)	4.31	10 (90%) 0 0	37, 53, 76, 78	0
2	K	11/12 (91%)	1.46	3 (27%) 1 1	22, 35, 42, 44	0
2	L	11/12 (91%)	4.70	11 (100%) 0 0	42, 59, 81, 85	0
2	M	11/12 (91%)	1.03	1 (9%) 15 17	22, 31, 39, 44	0
2	N	11/12 (91%)	1.54	3 (27%) 1 1	22, 35, 47, 52	0
2	O	11/12 (91%)	0.57	0 100 100	21, 27, 37, 41	0
2	P	11/12 (91%)	2.40	5 (45%) 0 0	28, 43, 55, 55	0
All	All	1000/1016 (98%)	0.07	49 (4%) 35 40	11, 16, 41, 85	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	11	LEU	8.7
2	L	12	LEU	7.9
2	J	5	LEU	7.5
2	J	12	LEU	7.1
2	J	4	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
2	L	10	LEU	6.2
2	L	5	LEU	5.5
2	J	3	LYS	4.7
2	P	10	LEU	4.5
2	J	8	LEU	4.4
2	L	7	LEU	4.3
2	L	4	LEU	4.2
2	J	10	LEU	3.9
2	P	7	LEU	3.9
2	K	11	LEU	3.9
2	L	6	LYS	3.7
2	N	12	LEU	3.7
2	L	9	LYS	3.6
1	H	70	ASN	3.6
2	I	3	LYS	3.6
2	I	12	LEU	3.5
2	L	3	LYS	3.4
1	A	70	ASN	3.4
2	P	11	LEU	3.3
2	J	11	LEU	3.3
2	J	9	LYS	3.2
2	N	10	LEU	3.2
1	E	33	ASN	2.9
2	I	9	LYS	2.9
1	B	70	ASN	2.9
2	I	5	LEU	2.9
2	J	6	LYS	2.8
1	G	33	ASN	2.8
2	I	10	LEU	2.8
2	K	10	LEU	2.6
2	K	12	LEU	2.5
2	P	4	LEU	2.5
2	M	11	LEU	2.4
2	I	6	LYS	2.3
2	P	6	LYS	2.3
2	L	2	LYS	2.1
2	J	7	LEU	2.1
1	E	70	ASN	2.1
1	G	34	ASN	2.1
2	N	5	LEU	2.0
2	I	11	LEU	2.0
2	L	8	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	33	ASN	2.0
1	C	70	ASN	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
4	ZDC	J	101	13/14	0.95	0.07	14,19,27,29	0
4	ZDC	P	101	13/14	0.95	0.07	13,17,22,24	0
4	ZDC	L	101	13/14	0.96	0.07	12,15,22,23	0
4	ZDC	N	101	13/14	0.96	0.06	13,17,23,24	0
4	ZDC	O	101	13/14	0.96	0.06	11,15,20,21	0
4	ZDC	I	101	13/14	0.96	0.06	12,16,18,21	0
4	ZDC	M	101	13/14	0.97	0.05	11,14,16,17	0
4	ZDC	K	101	13/14	0.97	0.06	12,15,20,21	0
3	CA	H	301	1/1	0.99	0.03	13,13,13,13	0
3	CA	H	302	1/1	0.99	0.03	13,13,13,13	0
3	CA	A	301	1/1	0.99	0.02	14,14,14,14	0
3	CA	B	301	1/1	0.99	0.02	14,14,14,14	0
3	CA	D	301	1/1	0.99	0.02	12,12,12,12	0
3	CA	D	302	1/1	0.99	0.03	14,14,14,14	0
3	CA	E	301	1/1	0.99	0.02	11,11,11,11	0
3	CA	F	301	1/1	0.99	0.03	14,14,14,14	0
3	CA	F	302	1/1	0.99	0.02	13,13,13,13	0
3	CA	G	302	1/1	0.99	0.02	12,12,12,12	0
3	CA	G	301	1/1	1.00	0.02	12,12,12,12	0
3	CA	B	302	1/1	1.00	0.01	13,13,13,13	0
3	CA	C	301	1/1	1.00	0.02	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	E	302	1/1	1.00	0.01	12,12,12,12	0
3	CA	C	302	1/1	1.00	0.02	14,14,14,14	0
3	CA	A	302	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.