



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 07:43 PM UTC

PDB ID : 1QNW / pdb_00001qnw
Title : lectin II from Ulex europaeus
Authors : Loris, R.; De Greve, H.; Dao-Thi, M.-H.; Messens, J.; Imberty, A.; Wyns, L.
Deposited on : 1999-10-22
Resolution : 2.35 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

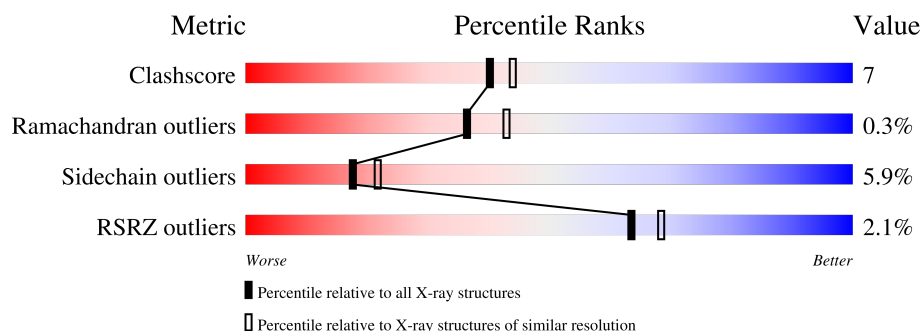
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	242	0% 79% 16% ..
1	B	242	2% 78% 19% ..
1	C	242	3% 75% 21% ..
1	D	242	2% 80% 17% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7433 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 CHITIN BINDING LECTIN, UEA-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	1
			1783	1145	285	351	2			
1	B	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			
1	C	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			
1	D	237	Total	C	N	O	S	0	0	1
			1795	1153	287	353	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASP	ALA	conflict	GB AF190633
A	62	ILE	THR	conflict	GB AF190633
A	106	GLY	SER	conflict	GB AF190633
A	112	SER	ASN	conflict	GB AF190633
A	191	GLY	GLU	conflict	GB AF190633
A	229	VAL	ILE	conflict	GB AF190633
B	25	ASP	ALA	conflict	GB AF190633
B	62	ILE	THR	conflict	GB AF190633
B	106	GLY	SER	conflict	GB AF190633
B	112	SER	ASN	conflict	GB AF190633
B	191	GLY	GLU	conflict	GB AF190633
B	229	VAL	ILE	conflict	GB AF190633
C	25	ASP	ALA	conflict	GB AF190633
C	62	ILE	THR	conflict	GB AF190633
C	106	GLY	SER	conflict	GB AF190633
C	112	SER	ASN	conflict	GB AF190633
C	191	GLY	GLU	conflict	GB AF190633
C	229	VAL	ILE	conflict	GB AF190633
D	25	ASP	ALA	conflict	GB AF190633
D	62	ILE	THR	conflict	GB AF190633
D	106	GLY	SER	conflict	GB AF190633

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	112	SER	ASN	conflict	GB AF190633
D	191	GLY	GLU	conflict	GB AF190633
D	229	VAL	ILE	conflict	GB AF190633

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

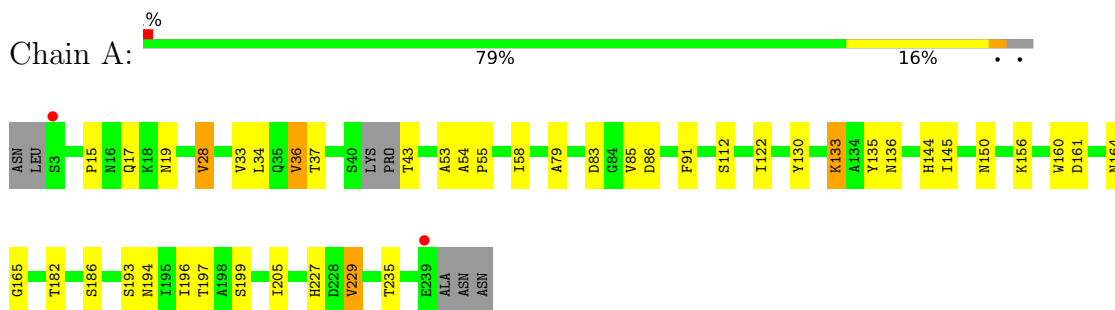
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	52	Total	O	0	0
			52	52		
5	C	51	Total	O	0	0
			51	51		
5	D	48	Total	O	0	0
			48	48		

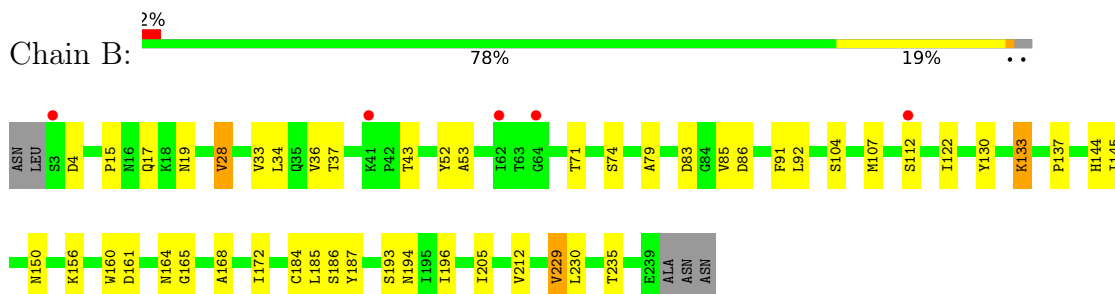
3 Residue-property plots [i](#)

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.

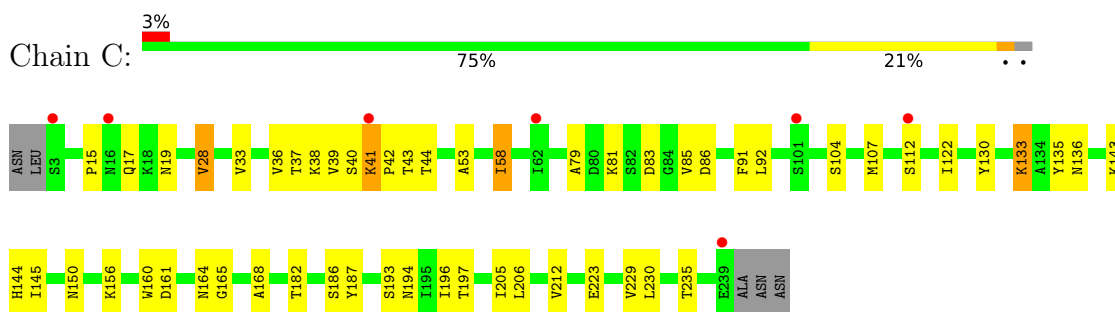
- Molecule 1: CHITIN BINDING LECTIN, UEA-II



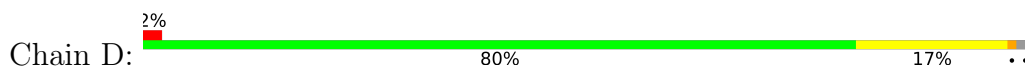
- Molecule 1: CHITIN BINDING LECTIN, UEA-II

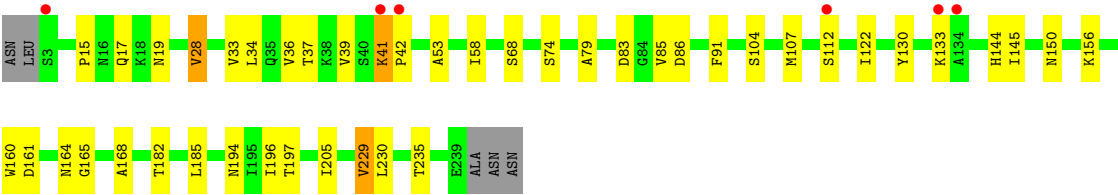


- Molecule 1: CHITIN BINDING LECTIN, UEA-II



- Molecule 1: CHITIN BINDING LECTIN, UEA-II





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.91Å 104.91Å 175.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.35) 97.0 (50.00-2.36)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.37Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.178 , 0.218 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7433	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: CA, NAG, MN

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	0.46	0/1827	0.94	4/2489 (0.2%)
1	B	0.50	0/1841	0.97	7/2511 (0.3%)
1	C	0.46	0/1841	0.95	6/2511 (0.2%)
1	D	0.47	0/1841	1.00	9/2511 (0.4%)
All	All	0.47	0/7350	0.97	26/10022 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	LYS	N-CA-C	10.07	124.67	112.38
1	D	41	LYS	CA-C-N	-8.02	110.37	120.23
1	D	41	LYS	C-N-CA	-8.02	110.37	120.23
1	D	42	PRO	N-CA-C	-7.08	99.38	110.50
1	D	205	ILE	N-CA-C	7.07	117.89	111.81
1	A	91	PHE	N-CA-C	6.56	118.74	108.96
1	A	53	ALA	N-CA-C	6.45	120.01	111.75
1	D	53	ALA	N-CA-C	6.45	120.01	111.75
1	B	53	ALA	N-CA-C	6.39	119.93	111.75
1	C	53	ALA	N-CA-C	6.30	119.81	111.75
1	B	91	PHE	N-CA-C	6.20	118.19	108.96
1	A	205	ILE	N-CA-C	5.94	116.92	111.81
1	B	205	ILE	N-CA-C	5.93	116.91	111.81
1	C	205	ILE	N-CA-C	5.86	116.85	111.81
1	D	91	PHE	N-CA-C	5.79	117.87	109.07
1	C	91	PHE	N-CA-C	5.60	117.30	108.96
1	B	43	THR	N-CA-C	5.44	117.75	110.35
1	A	144	HIS	N-CA-C	5.31	116.87	108.96
1	D	144	HIS	N-CA-C	5.18	116.69	108.96
1	D	68	SER	N-CA-C	-5.15	101.88	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LEU	N-CA-C	5.13	117.12	110.40
1	C	143	LYS	N-CA-C	-5.08	102.86	110.23
1	C	144	HIS	N-CA-C	5.05	116.48	108.96
1	B	52	TYR	N-CA-C	-5.04	102.41	109.96
1	B	144	HIS	N-CA-C	5.02	116.44	108.96
1	B	4	ASP	N-CA-C	5.00	117.35	110.35

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	1783	0	1721	22	0
1	B	1795	0	1731	23	0
1	C	1795	0	1731	32	0
1	D	1795	0	1731	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	50	0	0	0	0
5	B	52	0	0	1	0
5	C	51	0	0	1	0
5	D	48	0	0	0	0
All	All	7433	0	6966	93	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 7.

All (93) 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:D:182:THR:HG23	1:D:197:THR:HG22	1.71	0.72
1:B:79:ALA:H	1:B:164:ASN:HD21	1.37	0.72
1:C:133:LYS:HE3	1:C:133:LYS:HA	1.70	0.72
1:C:79:ALA:H	1:C:164:ASN:HD21	1.36	0.71
1:D:79:ALA:H	1:D:164:ASN:HD21	1.39	0.71
1:A:197:THR:HG23	1:C:193:SER:OG	1.91	0.70
1:A:79:ALA:H	1:A:164:ASN:HD21	1.41	0.67
1:C:182:THR:HG23	1:C:197:THR:HG22	1.78	0.64
1:A:193:SER:OG	1:C:197:THR:HG23	1.98	0.63
1:D:161:ASP:H	1:D:194:ASN:HD21	1.47	0.62
1:B:161:ASP:H	1:B:194:ASN:HD21	1.49	0.60
1:B:186:SER:CB	1:D:197:THR:HG21	2.31	0.60
1:B:186:SER:HB2	1:D:197:THR:HG21	1.84	0.59
1:A:182:THR:HG23	1:A:197:THR:HG22	1.83	0.58
1:C:161:ASP:H	1:C:194:ASN:HD21	1.50	0.58
1:A:161:ASP:H	1:A:194:ASN:HD21	1.52	0.58
1:D:15:PRO:HA	1:D:28:VAL:HG13	1.86	0.58
1:C:79:ALA:H	1:C:164:ASN:ND2	2.01	0.57
5:B:2042:HOH:O	1:D:196:ILE:HD12	2.04	0.56
1:A:15:PRO:HA	1:A:28:VAL:HG13	1.86	0.56
1:A:85:VAL:HG12	1:A:130:TYR:HB2	1.86	0.56
1:B:15:PRO:HA	1:B:28:VAL:HG13	1.87	0.55
1:C:133:LYS:HE3	1:C:133:LYS:CA	2.37	0.55
1:B:193:SER:OG	1:D:197:THR:HG23	2.07	0.54
1:B:133:LYS:HD3	1:B:137:PRO:HA	1.88	0.54
1:A:79:ALA:H	1:A:164:ASN:ND2	2.06	0.53
1:C:15:PRO:HA	1:C:28:VAL:HG13	1.90	0.53
1:D:85:VAL:HG12	1:D:130:TYR:HB2	1.91	0.53
1:C:17:GLN:HG2	1:C:19:ASN:OD1	2.10	0.52
1:C:85:VAL:HG12	1:C:130:TYR:HB2	1.91	0.52
1:B:17:GLN:HG2	1:B:19:ASN:OD1	2.11	0.51
1:B:79:ALA:H	1:B:164:ASN:ND2	2.06	0.51
1:A:196:ILE:HD12	5:C:2038:HOH:O	2.10	0.51
1:D:79:ALA:H	1:D:164:ASN:ND2	2.06	0.50
1:B:85:VAL:HG12	1:B:130:TYR:HB2	1.93	0.50
1:A:197:THR:HG21	1:C:186:SER:CB	2.42	0.49
1:C:156:LYS:HG2	1:C:196:ILE:HD11	1.94	0.49
1:A:17:GLN:HG2	1:A:19:ASN:OD1	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ILE:HG13	1:D:160:TRP:HB2	1.94	0.49
1:A:164:ASN:HD22	1:A:165:GLY:N	2.11	0.48
1:A:197:THR:HG21	1:C:186:SER:HB2	1.95	0.48
1:B:34:LEU:HB3	1:B:229:VAL:HG22	1.95	0.48
1:C:39:VAL:HG23	1:C:39:VAL:O	2.13	0.48
1:A:156:LYS:HG2	1:A:196:ILE:HD11	1.96	0.48
1:B:145:ILE:HG13	1:B:160:TRP:HB2	1.96	0.47
1:D:164:ASN:HD22	1:D:165:GLY:N	2.12	0.47
1:D:17:GLN:HG2	1:D:19:ASN:OD1	2.14	0.47
1:C:122:ILE:H	1:C:150:ASN:ND2	2.12	0.47
1:B:104:SER:OG	1:B:107:MET:HE2	2.16	0.46
1:B:161:ASP:H	1:B:194:ASN:ND2	2.13	0.46
1:C:135:TYR:C	1:C:136:ASN:HD22	2.23	0.46
1:C:104:SER:OG	1:C:107:MET:HE2	2.15	0.45
1:D:122:ILE:H	1:D:150:ASN:ND2	2.15	0.45
1:D:34:LEU:HB3	1:D:229:VAL:HG22	1.98	0.45
1:A:34:LEU:HB3	1:A:229:VAL:HG22	1.98	0.45
1:B:122:ILE:H	1:B:150:ASN:ND2	2.15	0.45
1:A:122:ILE:H	1:A:150:ASN:ND2	2.15	0.44
1:B:185:LEU:C	1:B:185:LEU:HD23	2.43	0.44
1:C:156:LYS:HE2	1:C:196:ILE:HD11	2.00	0.44
1:D:58:ILE:HD12	1:D:58:ILE:HA	1.88	0.44
1:C:145:ILE:HG13	1:C:160:TRP:HB2	2.00	0.43
1:D:104:SER:OG	1:D:107:MET:HE2	2.18	0.43
1:B:156:LYS:HG2	1:B:196:ILE:HD11	2.00	0.43
1:C:41:LYS:HA	1:C:43:THR:N	2.33	0.43
1:D:156:LYS:HE2	1:D:196:ILE:HD11	2.00	0.43
1:A:145:ILE:HG13	1:A:160:TRP:HB2	2.00	0.43
1:B:164:ASN:HD22	1:B:165:GLY:N	2.16	0.42
1:C:92:LEU:HG	1:C:212:VAL:HG12	2.00	0.42
1:A:133:LYS:HE3	1:A:133:LYS:HA	2.01	0.42
1:D:156:LYS:HG2	1:D:196:ILE:HD11	2.00	0.42
1:D:185:LEU:C	1:D:185:LEU:HD23	2.44	0.42
1:C:79:ALA:N	1:C:164:ASN:HD21	2.10	0.42
1:A:36:VAL:HG13	1:A:227:HIS:O	2.19	0.42
1:B:156:LYS:HE2	1:B:196:ILE:HD11	2.01	0.42
1:C:40:SER:O	1:C:41:LYS:C	2.62	0.42
1:B:92:LEU:HG	1:B:212:VAL:HG12	2.02	0.42
1:C:164:ASN:HD22	1:C:165:GLY:N	2.17	0.42
1:B:74:SER:HA	1:B:168:ALA:O	2.20	0.41
1:C:58:ILE:HD12	1:C:58:ILE:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ALA:HB2	1:C:187:TYR:CE1	2.55	0.41
1:D:79:ALA:N	1:D:164:ASN:HD21	2.12	0.41
1:C:39:VAL:O	1:C:39:VAL:CG2	2.69	0.41
1:D:74:SER:HA	1:D:168:ALA:O	2.21	0.41
1:A:135:TYR:C	1:A:136:ASN:HD22	2.28	0.41
1:A:186:SER:HB2	1:C:197:THR:HG21	2.02	0.41
1:B:71:THR:HG22	1:B:172:ILE:HB	2.02	0.41
1:C:38:LYS:HE3	1:C:44:THR:CG2	2.50	0.40
1:C:81:LYS:NZ	1:C:223:GLU:HG2	2.36	0.40
1:C:161:ASP:H	1:C:194:ASN:ND2	2.17	0.40
1:D:161:ASP:H	1:D:194:ASN:ND2	2.14	0.40
1:B:168:ALA:HB2	1:B:187:TYR:CE1	2.56	0.40
1:A:54:ALA:HA	1:A:55:PRO:HD3	1.96	0.40
1:D:39:VAL:O	1:D:39:VAL:HG23	2.21	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	231/242 (96%)	223 (96%)	8 (4%)	0	100	100
1	B	235/242 (97%)	225 (96%)	10 (4%)	0	100	100
1	C	235/242 (97%)	224 (95%)	9 (4%)	2 (1%)	14	14
1	D	235/242 (97%)	226 (96%)	8 (3%)	1 (0%)	30	34
All	All	936/968 (97%)	898 (96%)	35 (4%)	3 (0%)	36	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	41	LYS
1	C	41	LYS

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	197/205 (96%)	184 (93%)	13 (7%)	15	17
1	B	198/205 (97%)	186 (94%)	12 (6%)	17	20
1	C	198/205 (97%)	186 (94%)	12 (6%)	17	20
1	D	198/205 (97%)	188 (95%)	10 (5%)	21	26
All	All	791/820 (96%)	744 (94%)	47 (6%)	18	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	33	VAL
1	A	36	VAL
1	A	37	THR
1	A	43	THR
1	A	58	ILE
1	A	83	ASP
1	A	86	ASP
1	A	112	SER
1	A	133	LYS
1	A	199	SER
1	A	229	VAL
1	A	235	THR
1	B	28	VAL
1	B	33	VAL
1	B	36	VAL
1	B	37	THR
1	B	83	ASP
1	B	86	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	SER
1	B	133	LYS
1	B	184	CYS
1	B	229	VAL
1	B	230	LEU
1	B	235	THR
1	C	28	VAL
1	C	33	VAL
1	C	36	VAL
1	C	37	THR
1	C	58	ILE
1	C	83	ASP
1	C	86	ASP
1	C	112	SER
1	C	133	LYS
1	C	229	VAL
1	C	230	LEU
1	C	235	THR
1	D	28	VAL
1	D	33	VAL
1	D	36	VAL
1	D	37	THR
1	D	83	ASP
1	D	86	ASP
1	D	112	SER
1	D	229	VAL
1	D	230	LEU
1	D	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	57	GLN
1	A	120	ASN
1	A	150	ASN
1	A	164	ASN
1	A	194	ASN
1	A	220	ASN
1	A	227	HIS
1	A	237	ASN
1	B	35	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	120	ASN
1	B	150	ASN
1	B	164	ASN
1	B	194	ASN
1	B	220	ASN
1	B	227	HIS
1	B	237	ASN
1	C	35	GLN
1	C	120	ASN
1	C	150	ASN
1	C	164	ASN
1	C	194	ASN
1	C	220	ASN
1	C	227	HIS
1	C	237	ASN
1	D	35	GLN
1	D	120	ASN
1	D	150	ASN
1	D	164	ASN
1	D	194	ASN
1	D	220	ASN
1	D	227	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	NAG	A	401	1	14,14,15	0.71	0	17,19,21	1.25	3 (17%)
4	NAG	C	401	1	14,14,15	0.71	0	17,19,21	1.31	3 (17%)
4	NAG	B	401	1	14,14,15	0.81	1 (7%)	17,19,21	1.40	3 (17%)
4	NAG	D	401	1	14,14,15	0.67	0	17,19,21	1.12	1 (5%)

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	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
4	NAG	D	401	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)
4	B	401	NAG	C1-C2	2.35	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	NAG	C2-N2-C7	-3.17	118.66	122.90
4	A	401	NAG	C2-N2-C7	-3.10	118.75	122.90
4	C	401	NAG	C4-C3-C2	-3.03	106.57	111.02
4	D	401	NAG	C2-N2-C7	-2.77	119.18	122.90
4	B	401	NAG	C4-C3-C2	-2.76	106.98	111.02
4	C	401	NAG	O5-C1-C2	-2.27	107.78	111.29
4	C	401	NAG	C1-C2-N2	2.21	113.92	110.43
4	A	401	NAG	O5-C1-C2	-2.19	107.90	111.29
4	A	401	NAG	C4-C3-C2	-2.11	107.93	111.02
4	B	401	NAG	C1-C2-N2	2.01	113.61	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	NAG	C1-C2-N2-C7
4	C	401	NAG	C3-C2-N2-C7

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	235/242 (97%)	-0.19	2 (0%) 81 84	15, 25, 50, 69	0
1	B	237/242 (97%)	-0.14	5 (2%) 63 68	13, 24, 52, 67	0
1	C	237/242 (97%)	-0.12	7 (2%) 52 59	14, 26, 54, 69	0
1	D	237/242 (97%)	-0.11	6 (2%) 58 64	14, 25, 53, 68	0
All	All	946/968 (97%)	-0.14	20 (2%) 63 68	13, 25, 53, 69	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	SER	5.1
1	B	3	SER	4.8
1	A	3	SER	4.6
1	D	3	SER	4.5
1	D	134	ALA	3.8
1	B	62	ILE	3.7
1	C	239	GLU	2.9
1	D	41	LYS	2.8
1	C	62	ILE	2.7
1	B	41	LYS	2.5
1	D	42	PRO	2.4
1	D	112	SER	2.4
1	C	41	LYS	2.3
1	A	239	GLU	2.3
1	B	64	GLY	2.2
1	B	112	SER	2.2
1	C	112	SER	2.2
1	C	16	ASN	2.1
1	D	133	LYS	2.1
1	C	101	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](#)

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	NAG	C	401	14/15	0.62	0.22	58,69,87,90	0
4	NAG	D	401	14/15	0.66	0.17	67,75,80,80	0
4	NAG	A	401	14/15	0.72	0.18	64,72,75,76	0
4	NAG	B	401	14/15	0.73	0.20	50,61,66,66	0
3	CA	A	302	1/1	0.98	0.03	25,25,25,25	0
3	CA	D	308	1/1	0.99	0.03	25,25,25,25	0
2	MN	C	305	1/1	0.99	0.02	30,30,30,30	0
2	MN	A	301	1/1	0.99	0.03	37,37,37,37	0
3	CA	B	304	1/1	0.99	0.01	17,17,17,17	0
3	CA	C	306	1/1	0.99	0.02	30,30,30,30	0
2	MN	B	303	1/1	1.00	0.01	20,20,20,20	0
2	MN	D	307	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.