



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:08 AM BST

PDB ID : 4PLN  
Title : Crystal Structure of Chicken Netrin-1 (LN-LE3) complexed with mouse Neogenin (FN4-5)  
Authors : Xu, K.; Nikolov, D.B.  
Deposited on : 2014-05-18  
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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

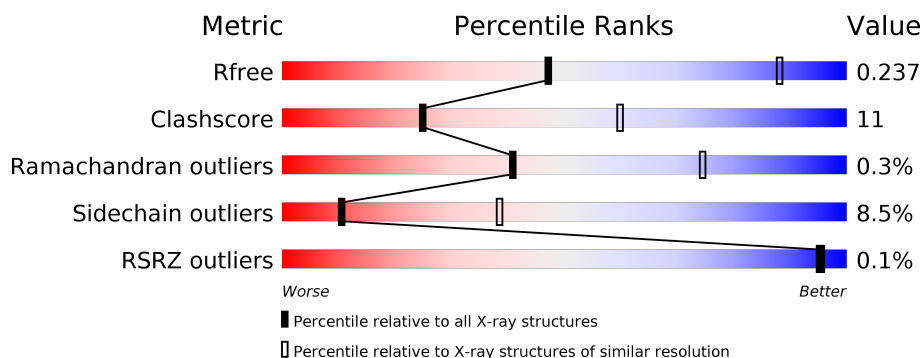
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	432	<div> <div style="width: 71%;"></div> <div style="width: 22%;"></div> <div style="width: 7%;"></div> <div style="width: 2%;"></div> </div> <div>71% 22% . .</div>
1	B	432	<div> <div style="width: 66%;"></div> <div style="width: 25%;"></div> <div style="width: 6%;"></div> <div style="width: 3%;"></div> </div> <div>66% 25% 6% .</div>
2	C	205	<div> <div style="width: 79%;"></div> <div style="width: 20%;"></div> <div style="width: 1%;"></div> </div> <div>79% 20% .</div>
2	D	205	<div> <div style="width: 74%;"></div> <div style="width: 23%;"></div> <div style="width: 3%;"></div> </div> <div>74% 23% .</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9826 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 Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3265	2005	607	615	38			
1	B	417	Total	C	N	O	S	0	0	0
			3271	2008	607	618	38			

- Molecule 2 is a protein called Neogenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	205	Total	C	N	O	S	0	0	0
			1604	1018	279	303	4			
2	D	204	Total	C	N	O	S	0	0	0
			1600	1016	278	302	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	763	GLY	-	expression tag	UNP P97798
C	764	SER	-	expression tag	UNP P97798
C	924	GLN	ASN	engineered mutation	UNP P97798
C	965	ALA	-	expression tag	UNP P97798
C	966	SER	-	expression tag	UNP P97798
C	967	GLY	-	expression tag	UNP P97798
D	763	GLY	-	expression tag	UNP P97798
D	764	SER	-	expression tag	UNP P97798
D	924	GLN	ASN	engineered mutation	UNP P97798
D	965	ALA	-	expression tag	UNP P97798
D	966	SER	-	expression tag	UNP P97798
D	967	GLY	-	expression tag	UNP P97798

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

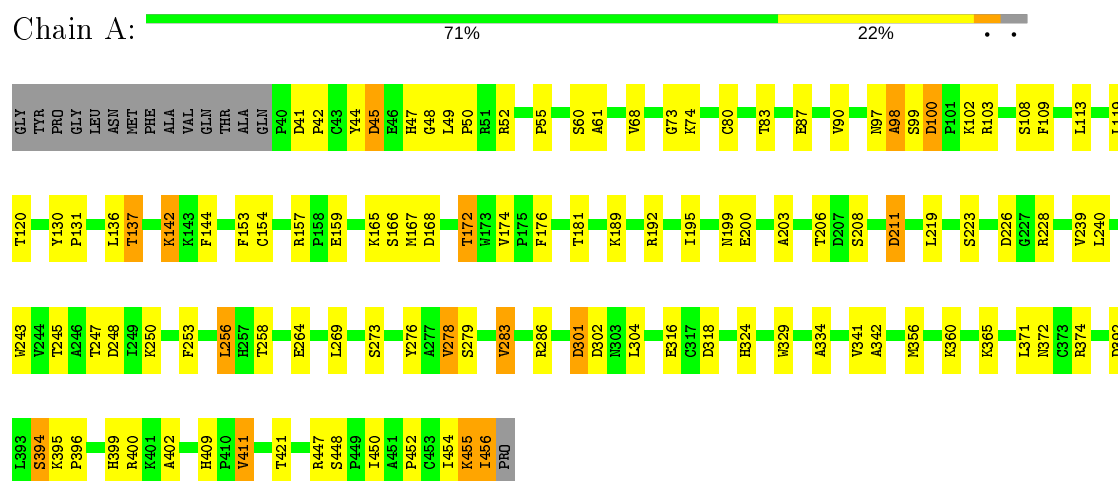
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

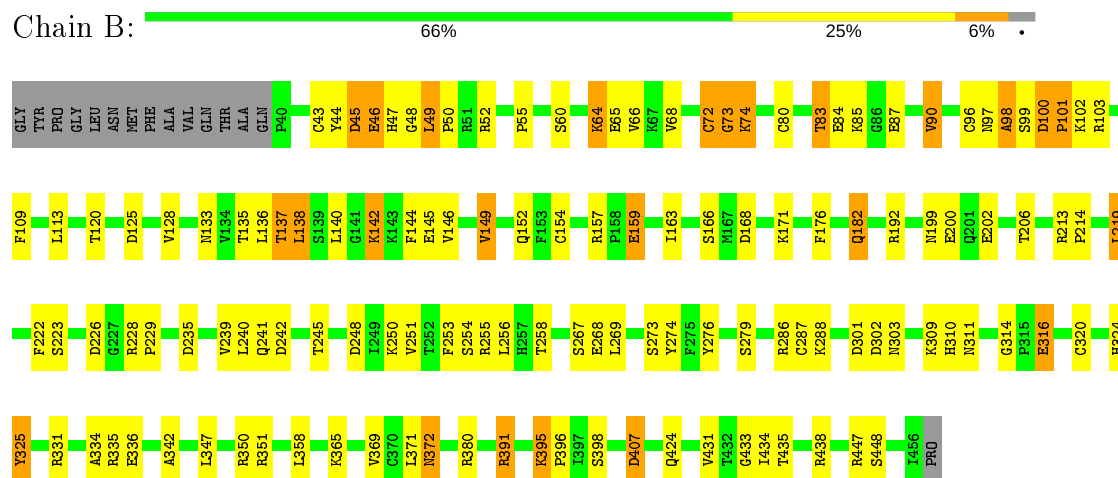
### 3 Residue-property plots

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.

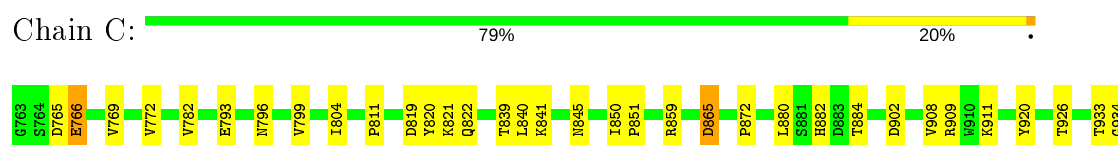
#### • Molecule 1: Netrin-1

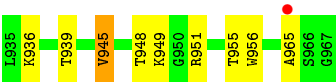


#### • Molecule 1: Netrin-1

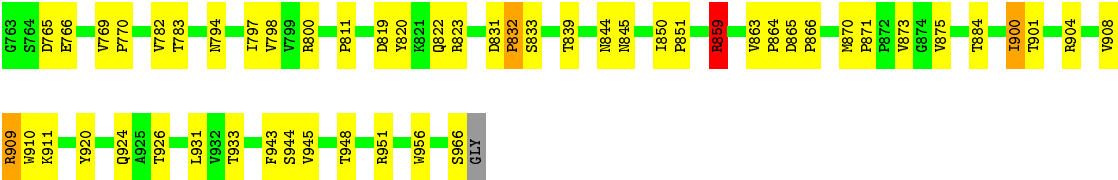


#### • Molecule 2: Neogenin





● Molecule 2: Neogenin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.07Å 130.21Å 126.04Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	49.95 – 3.20 49.95 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.95-3.20) 89.9 (49.95-3.19)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.90 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.196 , 0.239 0.197 , 0.237	Depositor DCC
$R_{free}$ test set	2000 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.44	0/3346	0.63	1/4529 (0.0%)
1	B	0.56	0/3352	0.62	4/4537 (0.1%)
2	C	0.34	0/1649	0.53	0/2259
2	D	0.51	0/1645	0.62	3/2254 (0.1%)
All	All	0.48	0/9992	0.61	8/13579 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	831	ASP	C-N-CD	6.54	142.14	128.40
1	A	100	ASP	C-N-CD	6.12	141.26	128.40
1	B	100	ASP	C-N-CD	-6.01	107.38	120.60
1	B	314	GLY	C-N-CD	5.95	140.90	128.40
2	D	859	ARG	C-N-CD	5.89	140.76	128.40
1	B	73	GLY	N-CA-C	5.20	126.11	113.10
1	B	138	LEU	CA-CB-CG	5.06	126.93	115.30
2	D	832	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.



All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ASP	Peptide
1	A	264	GLU	Peptide
1	B	74	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3265	0	3079	80	0
1	B	3271	0	3081	87	1
2	C	1604	0	1594	22	1
2	D	1600	0	1591	27	1
3	A	42	0	39	2	1
3	B	42	0	39	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9826	0	9423	208	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (208) 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:B:100:ASP:O	1:B:102:LYS:N	1.70	1.23
1:B:97:ASN:HD22	3:B:501:NAG:H83	1.26	1.01
1:B:142:LYS:NZ	1:B:316:GLU:OE2	1.98	0.97
1:B:97:ASN:ND2	3:B:501:NAG:H83	1.84	0.92
1:B:84:GLU:OE2	1:B:213:ARG:NH1	2.06	0.87
1:A:200:GLU:O	1:A:228:ARG:NH1	2.12	0.82
1:A:374:ARG:NH2	1:B:46:GLU:OE2	2.12	0.81
1:B:166:SER:HB3	1:B:248:ASP:HB2	1.64	0.78
1:B:371:LEU:O	1:B:372:ASN:ND2	2.17	0.77
1:A:166:SER:HB3	1:A:248:ASP:HB2	1.68	0.76
1:B:145:GLU:OE2	1:B:331:ARG:NH2	2.22	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLU:OE2	1:B:255:ARG:NH2	2.23	0.70
1:B:52:ARG:NH1	1:B:235:ASP:OD1	2.26	0.69
1:B:200:GLU:O	1:B:228:ARG:NH1	2.26	0.69
1:A:400:ARG:HH12	1:B:336:GLU:HA	1.59	0.68
1:A:400:ARG:NH1	1:B:335:ARG:O	2.26	0.68
1:B:245:THR:HG21	1:B:288:LYS:HZ3	1.58	0.67
2:D:800:ARG:HG2	2:D:800:ARG:HH11	1.58	0.67
1:A:97:ASN:OD1	3:A:501:NAG:N2	2.27	0.67
1:A:97:ASN:O	1:A:99:SER:N	2.30	0.64
1:A:73:GLY:HA3	1:A:98:ALA:HB2	1.79	0.64
2:C:804:ILE:HG12	2:C:840:LEU:HD23	1.80	0.64
1:B:324:HIS:HA	1:B:342:ALA:HA	1.81	0.63
1:B:391:ARG:NH1	1:B:395:LYS:O	2.32	0.63
1:A:192:ARG:NH2	1:A:208:SER:OG	2.33	0.62
1:A:73:GLY:CA	1:A:98:ALA:HB2	2.29	0.61
1:A:400:ARG:HH11	1:B:336:GLU:CD	2.04	0.61
1:A:159:GLU:OE2	1:A:181:THR:HB	2.01	0.61
1:A:400:ARG:NH1	1:B:336:GLU:HA	2.15	0.60
1:A:223:SER:HB3	1:A:226:ASP:HB2	1.82	0.60
1:A:454:ILE:HG12	1:A:455:LYS:H	1.66	0.60
2:D:859:ARG:O	2:D:859:ARG:HD2	2.01	0.60
1:A:168:ASP:OD2	1:A:172:THR:HG23	2.01	0.60
1:B:256:LEU:HD13	1:B:274:TYR:HB3	1.84	0.59
1:B:371:LEU:C	1:B:372:ASN:HD22	2.04	0.59
1:B:100:ASP:C	1:B:102:LYS:H	1.94	0.59
1:A:189:LYS:HE2	1:A:203:ALA:O	2.03	0.59
1:B:168:ASP:OD1	1:B:171:LYS:HB2	2.03	0.59
1:A:61:ALA:HB2	1:A:283:VAL:HG12	1.85	0.58
2:C:865:ASP:N	2:C:865:ASP:OD1	2.36	0.58
2:C:819:ASP:OD1	2:C:822:GLN:HG2	2.03	0.58
1:A:409:HIS:CE1	1:A:411:VAL:HG13	2.38	0.58
2:D:900:ILE:HD11	2:D:904:ARG:HD2	1.85	0.58
1:B:157:ARG:NH2	1:B:219:LEU:O	2.37	0.57
1:B:309:LYS:O	1:B:310:HIS:HB2	2.04	0.57
2:D:766:GLU:OE2	2:D:845:ASN:HB2	2.04	0.57
2:D:870:MET:SD	2:D:871:PRO:HD2	2.44	0.57
1:A:68:VAL:HG12	1:A:136:LEU:HD22	1.86	0.57
1:A:97:ASN:HD22	1:A:100:ASP:HB2	1.70	0.57
2:C:902:ASP:OD2	2:C:949:LYS:HD2	2.04	0.57
1:B:52:ARG:CZ	1:B:334:ALA:HB2	2.35	0.56
1:A:142:LYS:HB2	1:A:304:LEU:HD23	1.85	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:O	1:A:102:LYS:N	2.38	0.56
1:B:245:THR:HG21	1:B:288:LYS:NZ	2.21	0.55
2:C:908:VAL:HG22	2:C:945:VAL:HB	1.87	0.55
1:A:74:LYS:HG3	1:A:98:ALA:CB	2.37	0.55
1:B:163:ILE:HG12	1:B:251:VAL:HG12	1.89	0.55
1:B:84:GLU:CD	1:B:213:ARG:HH11	2.09	0.55
1:A:73:GLY:C	1:A:98:ALA:HB2	2.26	0.55
1:A:154:CYS:SG	1:A:279:SER:HB3	2.47	0.54
2:D:819:ASP:OD1	2:D:822:GLN:HG2	2.08	0.54
2:D:820:TYR:O	2:D:823:ARG:NH2	2.41	0.54
1:A:157:ARG:NH2	1:A:211:ASP:O	2.41	0.53
1:A:399:HIS:HD2	1:A:400:ARG:H	1.55	0.53
1:B:83:THR:HB	1:B:85:LYS:HZ2	1.73	0.53
1:B:223:SER:HB3	1:B:226:ASP:HB2	1.91	0.53
1:B:159:GLU:OE2	1:B:255:ARG:NE	2.41	0.53
2:C:884:THR:HG22	2:C:933:THR:HA	1.90	0.53
1:B:100:ASP:O	1:B:103:ARG:N	2.42	0.52
1:B:142:LYS:HE2	1:B:287:CYS:SG	2.49	0.52
2:D:908:VAL:HG22	2:D:945:VAL:HG22	1.91	0.52
1:B:68:VAL:HG12	1:B:136:LEU:HG	1.92	0.52
1:B:100:ASP:O	1:B:102:LYS:CA	2.56	0.52
2:C:872:PRO:HG2	2:C:945:VAL:HG22	1.90	0.52
1:A:395:LYS:HD2	1:A:399:HIS:CE1	2.45	0.52
1:A:324:HIS:HA	1:A:342:ALA:HA	1.90	0.51
1:A:109:PHE:CD2	1:A:120:THR:HB	2.45	0.51
1:B:199:ASN:ND2	1:B:202:GLU:OE2	2.43	0.51
1:A:399:HIS:HD2	1:A:400:ARG:N	2.08	0.51
1:A:142:LYS:NZ	1:A:316:GLU:HG3	2.26	0.51
1:B:253:PHE:HB3	1:B:276:TYR:CE1	2.46	0.51
1:B:60:SER:O	1:B:64:LYS:NZ	2.39	0.51
2:C:765:ASP:N	2:C:796:ASN:O	2.43	0.50
1:A:411:VAL:HG23	1:A:452:PRO:HB3	1.93	0.50
1:B:434:ILE:HG23	1:B:435:THR:HG23	1.92	0.50
1:A:400:ARG:NH1	1:B:336:GLU:CD	2.65	0.50
2:C:909:ARG:HD2	2:C:920:TYR:CD1	2.46	0.50
3:B:501:NAG:H83	3:B:501:NAG:C1	2.41	0.50
1:A:74:LYS:HG3	1:A:98:ALA:HB3	1.94	0.50
1:B:152:GLN:O	1:B:279:SER:N	2.43	0.50
2:D:863:VAL:N	2:D:864:PRO:HD2	2.26	0.50
2:C:820:TYR:OH	2:C:821:LYS:NZ	2.45	0.50
1:B:245:THR:CG2	1:B:288:LYS:NZ	2.75	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASP:C	1:A:102:LYS:H	2.16	0.49
1:A:301:ASP:N	1:A:301:ASP:OD1	2.43	0.49
1:A:97:ASN:C	1:A:99:SER:H	2.15	0.49
1:A:144:PHE:O	1:A:245:THR:HA	2.12	0.49
1:A:55:PRO:O	1:A:286:ARG:NH2	2.45	0.49
1:A:73:GLY:HA3	1:A:98:ALA:N	2.28	0.49
1:A:153:PHE:HA	1:A:278:VAL:HA	1.95	0.49
1:B:60:SER:HB3	1:B:144:PHE:CE2	2.48	0.48
1:A:256:LEU:HD22	1:A:276:TYR:CZ	2.49	0.48
1:B:100:ASP:OD2	1:B:103:ARG:HG2	2.13	0.48
2:D:910:TRP:HB3	2:D:943:PHE:CD1	2.49	0.48
1:A:192:ARG:NH2	1:A:208:SER:HG	2.10	0.48
1:B:100:ASP:O	1:B:101:PRO:C	2.47	0.48
1:A:80:CYS:HB2	1:A:273:SER:HB3	1.96	0.48
1:B:47:HIS:HA	1:B:48:GLY:HA2	1.66	0.48
1:B:149:VAL:HG13	1:B:222:PHE:HD2	1.78	0.48
1:A:52:ARG:CZ	1:A:334:ALA:HB2	2.44	0.48
1:B:213:ARG:HA	1:B:214:PRO:C	2.34	0.48
2:C:772:VAL:HG12	2:C:850:ILE:HB	1.95	0.48
1:B:74:LYS:NZ	1:B:125:ASP:OD2	2.37	0.47
1:A:392:ASP:OD1	1:A:394:SER:HB3	2.14	0.47
1:B:109:PHE:CG	1:B:120:THR:HB	2.50	0.47
1:B:310:HIS:O	1:B:311:ASN:HB2	2.14	0.47
2:D:884:THR:HG22	2:D:933:THR:HA	1.96	0.47
1:A:324:HIS:CE1	1:A:342:ALA:HB2	2.49	0.47
1:A:137:THR:HB	1:A:250:LYS:NZ	2.30	0.47
2:D:800:ARG:NH1	2:D:800:ARG:HG2	2.28	0.47
1:B:347:LEU:HD12	1:B:398:SER:HB2	1.96	0.47
1:A:109:PHE:CG	1:A:120:THR:HB	2.51	0.46
2:D:770:PRO:HD3	2:D:844:ASN:ND2	2.31	0.46
2:C:882:HIS:HA	2:C:965:ALA:H	1.80	0.46
2:C:766:GLU:OE2	2:C:845:ASN:HB2	2.16	0.46
2:D:911:LYS:HB3	2:D:920:TYR:CD1	2.51	0.46
1:A:47:HIS:HA	1:A:48:GLY:HA2	1.66	0.46
2:D:909:ARG:HD3	2:D:920:TYR:CE1	2.51	0.45
1:B:302:ASP:C	1:B:302:ASP:OD1	2.54	0.45
1:A:356:MET:O	1:A:360:LYS:HG2	2.17	0.45
1:A:142:LYS:HZ3	1:A:316:GLU:HG3	1.80	0.45
1:B:424:GLN:NE2	1:B:433:GLY:O	2.49	0.45
1:A:167:MET:HG2	1:A:245:THR:O	2.17	0.45
1:A:165:LYS:NZ	1:A:243:TRP:O	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HB	1:B:250:LYS:NZ	2.32	0.45
1:B:228:ARG:HA	1:B:229:PRO:HD3	1.75	0.45
1:B:73:GLY:HA3	1:B:98:ALA:HB2	1.97	0.45
2:D:850:ILE:HA	2:D:851:PRO:HD3	1.73	0.45
1:A:371:LEU:O	1:A:372:ASN:OD1	2.35	0.44
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.79	0.44
1:A:399:HIS:CD2	1:A:400:ARG:N	2.84	0.44
2:D:909:ARG:HG2	2:D:956:TRP:CZ3	2.53	0.44
1:B:44:TYR:HA	1:B:50:PRO:HA	1.98	0.44
1:B:80:CYS:HB2	1:B:273:SER:HB3	2.00	0.44
1:A:52:ARG:NH2	1:A:334:ALA:HB2	2.32	0.44
1:B:43:CYS:HB3	1:B:310:HIS:HE2	1.82	0.44
1:B:55:PRO:O	1:B:286:ARG:NH2	2.50	0.44
2:C:820:TYR:CZ	2:C:821:LYS:NZ	2.86	0.44
2:D:864:PRO:HA	2:D:865:ASP:HA	1.61	0.44
1:A:399:HIS:HB3	1:A:402:ALA:HB2	2.00	0.44
1:B:303:ASN:OD1	1:B:303:ASN:N	2.51	0.44
1:B:407:ASP:OD1	1:B:407:ASP:N	2.40	0.43
1:B:97:ASN:O	1:B:99:SER:N	2.52	0.43
1:A:60:SER:HB3	1:A:144:PHE:CZ	2.53	0.43
1:B:133:ASN:HB3	1:B:254:SER:HA	1.99	0.43
1:A:396:PRO:HB3	1:B:365:LYS:HB2	2.00	0.43
2:D:782:VAL:HG22	2:D:859:ARG:O	2.18	0.43
2:D:811:PRO:HB2	2:D:839:THR:HG22	2.00	0.43
1:A:168:ASP:O	1:A:247:THR:OG1	2.37	0.43
1:A:45:ASP:N	1:A:49:LEU:O	2.42	0.43
2:D:866:PRO:HB3	2:D:951:ARG:NH1	2.34	0.43
1:B:241:GLN:O	1:B:245:THR:OG1	2.37	0.43
1:B:320:CYS:HB2	1:B:325:TYR:HD2	1.84	0.43
1:B:45:ASP:N	1:B:49:LEU:O	2.41	0.43
1:B:135:THR:HG22	1:B:137:THR:HG22	2.01	0.43
2:D:909:ARG:HD3	2:D:920:TYR:CD1	2.54	0.43
1:B:350:ARG:O	1:B:351:ARG:HG3	2.17	0.42
1:B:182:GLN:HB3	1:B:182:GLN:HE21	1.64	0.42
1:B:269:LEU:HD23	1:B:269:LEU:HA	1.90	0.42
2:D:765:ASP:O	2:D:798:VAL:HG12	2.19	0.42
1:A:253:PHE:HB3	1:A:276:TYR:CE1	2.54	0.42
2:C:841:LYS:HE2	2:C:851:PRO:HG3	2.02	0.42
2:C:909:ARG:HG2	2:C:956:TRP:CZ3	2.54	0.42
2:D:794:ASN:OD1	2:D:797:ILE:HG12	2.20	0.42
1:A:44:TYR:HA	1:A:50:PRO:HA	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ASN:O	1:A:199:ASN:OD1	2.37	0.42
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.85	0.42
1:A:318:ASP:HA	1:A:329:TRP:CZ2	2.54	0.42
1:A:113:LEU:HD13	2:C:850:ILE:HG12	2.01	0.42
1:A:100:ASP:C	1:A:102:LYS:N	2.72	0.41
1:B:154:CYS:SG	1:B:279:SER:OG	2.77	0.41
1:B:159:GLU:OE2	1:B:255:ARG:CZ	2.67	0.41
1:B:424:GLN:HG2	1:B:434:ILE:HD12	2.02	0.41
1:A:153:PHE:CD2	1:A:157:ARG:HG2	2.54	0.41
1:B:369:VAL:HG12	1:B:380:ARG:HG3	2.02	0.41
2:D:909:ARG:NH1	2:D:956:TRP:NE1	2.68	0.41
2:C:811:PRO:HB2	2:C:839:THR:HG22	2.01	0.41
1:A:365:LYS:HB2	1:B:396:PRO:HB3	2.03	0.41
2:C:955:THR:OG1	2:C:956:TRP:N	2.54	0.41
1:B:113:LEU:HD13	2:D:850:ILE:HG12	2.02	0.41
1:B:83:THR:HB	1:B:90:VAL:HG13	2.02	0.41
1:B:60:SER:HB2	1:B:140:LEU:HD22	2.03	0.41
2:C:933:THR:OG1	2:C:934:GLY:N	2.53	0.41
2:D:909:ARG:NH1	2:D:956:TRP:CD1	2.88	0.41
1:A:41:ASP:HA	1:A:42:PRO:HD2	1.89	0.41
1:A:97:ASN:CG	3:A:501:NAG:HN2	2.16	0.41
1:B:166:SER:OG	1:B:168:ASP:O	2.28	0.41
1:A:119:LEU:HD22	1:A:279:SER:HB2	2.03	0.40
3:B:501:NAG:C1	3:B:501:NAG:C8	2.99	0.40
1:A:100:ASP:OD2	1:A:103:ARG:HD3	2.20	0.40
2:C:911:LYS:HB3	2:C:920:TYR:CD1	2.56	0.40
1:A:130:TYR:HA	1:A:131:PRO:HA	1.75	0.40
1:A:456:ILE:H	1:A:456:ILE:HG12	1.64	0.40
1:A:60:SER:HB3	1:A:144:PHE:CE1	2.57	0.40
1:B:137:THR:HB	1:B:250:LYS:HZ3	1.87	0.40
1:B:74:LYS:HG2	1:B:74:LYS:H	1.69	0.40
1:B:72:CYS:HB2	1:B:96:CYS:HB3	2.01	0.40
2:C:936:LYS:O	2:C:939:THR:OG1	2.40	0.40

All (2) 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)
2:D:924:GLN:OE1	3:A:501:NAG:O7[2_545]	1.84	0.36
1:B:268:GLU:OE2	2:C:951:ARG:NE[2_645]	2.17	0.03

## 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	415/432 (96%)	395 (95%)	19 (5%)	1 (0%)	47	79
1	B	415/432 (96%)	390 (94%)	23 (6%)	2 (0%)	29	67
2	C	203/205 (99%)	197 (97%)	5 (2%)	1 (0%)	29	67
2	D	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
All	All	1235/1274 (97%)	1178 (95%)	53 (4%)	4 (0%)	41	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	PRO
1	A	98	ALA
1	B	98	ALA
2	C	782	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/378 (97%)	335 (92%)	30 (8%)	11	41
1	B	366/378 (97%)	328 (90%)	38 (10%)	7	28
2	C	181/181 (100%)	171 (94%)	10 (6%)	21	57
2	D	181/181 (100%)	166 (92%)	15 (8%)	11	40
All	All	1093/1118 (98%)	1000 (92%)	93 (8%)	10	38

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASP
1	A	83	THR
1	A	87	GLU
1	A	90	VAL
1	A	108	SER
1	A	137	THR
1	A	142	LYS
1	A	172	THR
1	A	174	VAL
1	A	176	PHE
1	A	195	ILE
1	A	206	THR
1	A	219	LEU
1	A	239	VAL
1	A	240	LEU
1	A	256	LEU
1	A	258	THR
1	A	278	VAL
1	A	283	VAL
1	A	301	ASP
1	A	302	ASP
1	A	341	VAL
1	A	394	SER
1	A	411	VAL
1	A	421	THR
1	A	447	ARG
1	A	448	SER
1	A	450	ILE
1	A	455	LYS
1	A	456	ILE
1	B	45	ASP
1	B	46	GLU
1	B	49	LEU
1	B	64	LYS
1	B	65	GLU
1	B	66	VAL
1	B	72	CYS
1	B	83	THR
1	B	87	GLU
1	B	90	VAL
1	B	128	VAL
1	B	137	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	138	LEU
1	B	142	LYS
1	B	146	VAL
1	B	149	VAL
1	B	159	GLU
1	B	176	PHE
1	B	182	GLN
1	B	192	ARG
1	B	206	THR
1	B	219	LEU
1	B	239	VAL
1	B	240	LEU
1	B	242	ASP
1	B	258	THR
1	B	267	SER
1	B	301	ASP
1	B	316	GLU
1	B	325	TYR
1	B	372	ASN
1	B	391	ARG
1	B	395	LYS
1	B	407	ASP
1	B	431	VAL
1	B	438	ARG
1	B	447	ARG
1	B	448	SER
2	C	766	GLU
2	C	769	VAL
2	C	793	GLU
2	C	799	VAL
2	C	859	ARG
2	C	865	ASP
2	C	880	LEU
2	C	926	THR
2	C	945	VAL
2	C	948	THR
2	D	769	VAL
2	D	783	THR
2	D	832	PRO
2	D	833	SER
2	D	859	ARG
2	D	873	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	875	VAL
2	D	900	ILE
2	D	901	THR
2	D	909	ARG
2	D	926	THR
2	D	931	LEU
2	D	944	SER
2	D	948	THR
2	D	966	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	HIS
1	B	372	ASN
2	C	897	HIS
2	D	861	HIS
2	D	892	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
3	NAG	B	501	1	14,14,15	1.06	0	17,19,21	2.52	6 (35%)
3	NAG	A	503	1	14,14,15	0.36	0	17,19,21	0.33	0
3	NAG	B	503	1	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	A	501	1	14,14,15	1.15	1 (7%)	17,19,21	2.70	10 (58%)
3	NAG	A	502	1	14,14,15	0.62	0	17,19,21	1.09	1 (5%)
3	NAG	B	502	1	14,14,15	0.29	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	501	1	-	3/6/23/26	0/1/1/1
3	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	NAG	B	503	1	-	2/6/23/26	0/1/1/1
3	NAG	A	501	1	-	5/6/23/26	0/1/1/1
3	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	C1-C2	2.00	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAG	C1-O5-C5	7.03	121.72	112.19
3	A	501	NAG	O5-C5-C6	-4.98	99.39	107.20
3	A	501	NAG	C1-O5-C5	4.38	118.13	112.19
3	B	501	NAG	C4-C3-C2	-4.17	104.91	111.02
3	A	501	NAG	O5-C1-C2	-4.15	104.73	111.29
3	A	501	NAG	O6-C6-C5	-3.62	98.88	111.29
3	B	501	NAG	O5-C1-C2	-3.49	105.77	111.29
3	A	501	NAG	C1-C2-N2	-3.08	105.23	110.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	O3-C3-C2	-3.07	103.12	109.47
3	A	501	NAG	C2-N2-C7	-2.80	118.91	122.90
3	B	501	NAG	C8-C7-N2	2.78	120.80	116.10
3	A	501	NAG	C6-C5-C4	-2.71	106.66	113.00
3	B	501	NAG	C6-C5-C4	-2.63	106.85	113.00
3	B	501	NAG	O3-C3-C4	-2.56	104.42	110.35
3	A	501	NAG	O3-C3-C4	-2.34	104.94	110.35
3	A	502	NAG	C1-O5-C5	2.23	115.21	112.19
3	A	501	NAG	O7-C7-N2	-2.14	118.01	121.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAG	C3-C2-N2-C7
3	A	501	NAG	C3-C2-N2-C7
3	A	501	NAG	C8-C7-N2-C2
3	A	501	NAG	O7-C7-N2-C2
3	A	503	NAG	O5-C5-C6-O6
3	A	502	NAG	O5-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6
3	A	503	NAG	C4-C5-C6-O6
3	B	503	NAG	C4-C5-C6-O6
3	B	502	NAG	C4-C5-C6-O6
3	B	501	NAG	C8-C7-N2-C2
3	B	501	NAG	O7-C7-N2-C2
3	A	502	NAG	C4-C5-C6-O6
3	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	NAG	4	0
3	A	501	NAG	2	1

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	417/432 (96%)	-0.34	0 100 100	25, 46, 78, 129	0
1	B	417/432 (96%)	-0.34	0 100 100	22, 46, 76, 119	0
2	C	205/205 (100%)	-0.19	1 (0%) 91 86	27, 55, 93, 131	0
2	D	204/205 (99%)	-0.20	0 100 100	29, 56, 85, 110	0
All	All	1243/1274 (97%)	-0.29	1 (0%) 95 95	22, 48, 83, 131	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	965	ALA	2.5

### 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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	NAG	A	502	14/15	0.85	0.27	62,85,100,103	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	504	1/1	0.86	0.17	47,47,47,47	0
3	NAG	A	501	14/15	0.87	0.22	45,60,80,93	0
3	NAG	B	502	14/15	0.88	0.30	56,92,104,108	0
3	NAG	B	501	14/15	0.94	0.19	55,59,68,70	0
4	CA	B	504	1/1	0.95	0.15	40,40,40,40	0
3	NAG	B	503	14/15	0.96	0.14	28,36,52,55	0
3	NAG	A	503	14/15	0.96	0.17	30,43,57,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.