



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PLO  
Title : Crystal Structure of chicken Netrin-1 (LN-LE3) in complex with mouse DCC (FN4-5)  
Authors : Xu, K.; Nikolov, D.B.  
Deposited on : 2014-05-18  
Resolution : 2.90 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

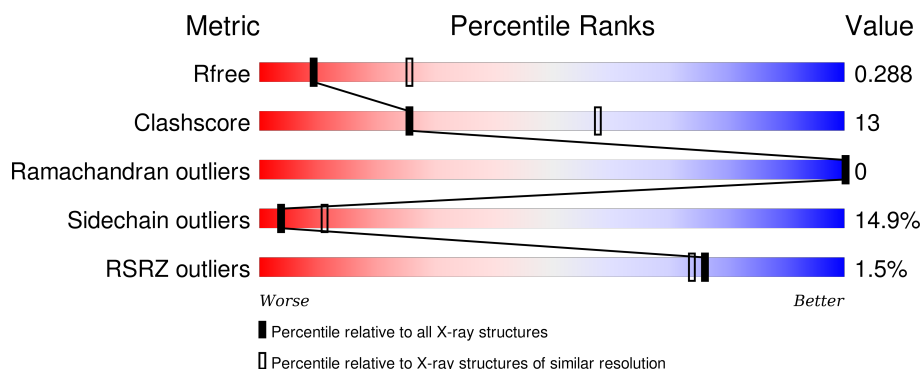
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	B	206	<div> <div> <div>2%</div> <div>66%</div> <div>26%</div> <div>7%</div> </div> </div>
2	A	432	<div> <div>2%</div> <div>59%</div> <div>32%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	502	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4868 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 receptor DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	192	Total	C	N	O	S	0	0	0
			1498	939	259	294	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	719	GLY	-	expression tag	UNP P70211
B	720	ALA	-	expression tag	UNP P70211
B	923	SER	-	expression tag	UNP P70211
B	924	GLY	-	expression tag	UNP P70211

- Molecule 2 is a protein called Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	412	Total	C	N	O	S	0	0	0
			3230	1987	601	604	38			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

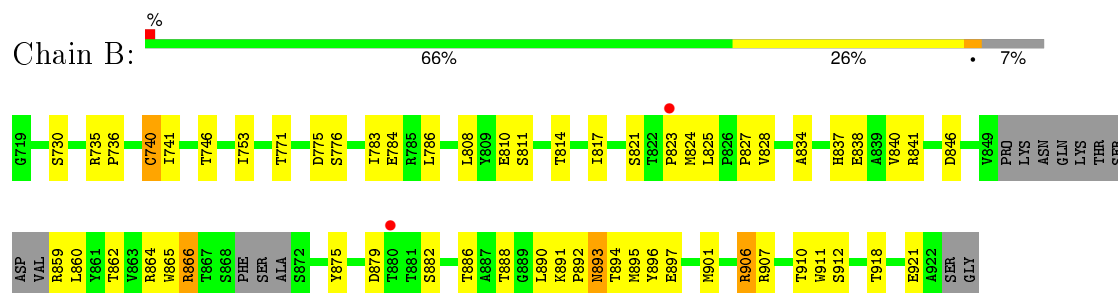
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	16	Total	O	0	0
			16	16		
6	A	56	Total	O	0	0
			56	56		

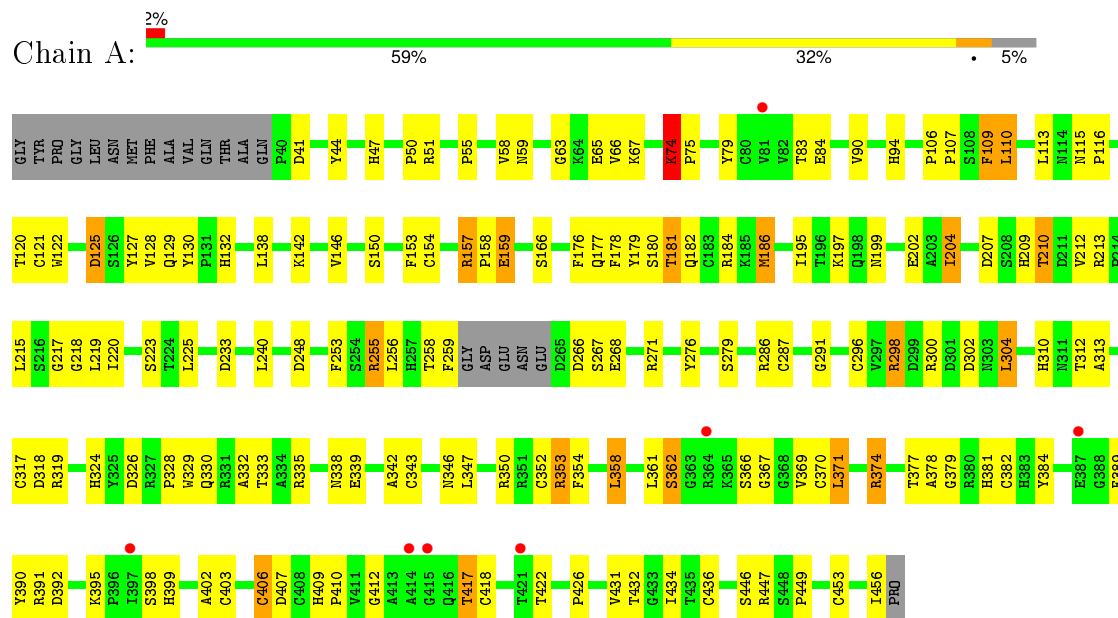
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 receptor DCC



#### • Molecule 2: Netrin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.48Å 72.94Å 285.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.90 48.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.75-2.90) 88.7 (48.75-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.224 , 0.288 0.224 , 0.288	Depositor DCC
$R_{free}$ test set	1868 reflections (8.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 22820 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, SO4

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	B	0.39	0/1533	0.61	0/2092
2	A	0.58	2/3310 (0.1%)	0.73	3/4479 (0.1%)
All	All	0.52	2/4843 (0.0%)	0.70	3/6571 (0.0%)

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
2	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	109	PHE	C-O	-6.85	1.10	1.23
2	A	44	TYR	CE1-CZ	-5.62	1.31	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	115	ASN	C-N-CD	6.37	141.78	128.40
2	A	41	ASP	C-N-CD	5.90	140.79	128.40
2	A	116	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	63	GLY	Peptide
2	A	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	B	1498	0	1462	25	0
2	A	3230	0	3054	92	0
3	A	42	0	39	0	0
4	A	25	0	0	3	0
5	A	1	0	0	0	0
6	A	56	0	0	7	0
6	B	16	0	0	0	0
All	All	4868	0	4555	117	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 13.

All (117) 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:A:166:SER:HB3	2:A:248:ASP:HB2	1.62	0.81
2:A:125:ASP:OD1	2:A:125:ASP:N	2.13	0.78
2:A:391:ARG:NH2	2:A:402:ALA:O	2.21	0.73
2:A:159:GLU:OE1	2:A:181:THR:OG1	2.06	0.71
2:A:158:PRO:HB3	2:A:276:TYR:HE1	1.55	0.71
1:B:837:HIS:HB2	1:B:892:PRO:HB3	1.72	0.70
2:A:199:ASN:ND2	2:A:202:GLU:OE2	2.24	0.69
2:A:110:LEU:HD13	2:A:122:TRP:HB3	1.75	0.68
1:B:834:ALA:HA	1:B:840:VAL:HG22	1.78	0.66
2:A:159:GLU:HA	2:A:210:THR:HG22	1.78	0.65
2:A:374:ARG:NH1	6:A:616:HOH:O	2.29	0.65
2:A:406:CYS:SG	2:A:418:CYS:N	2.70	0.65
1:B:906:ARG:O	1:B:907:ARG:NH1	2.30	0.64
2:A:350:ARG:NE	4:A:507:SO4:O2	2.31	0.63
2:A:352:CYS:SG	6:A:653:HOH:O	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:GLU:HG3	2:A:255:ARG:HB3	1.80	0.61
2:A:207:ASP:O	2:A:210:THR:OG1	2.15	0.61
2:A:379:GLY:HA2	2:A:382:CYS:H	1.66	0.61
1:B:740:CYS:SG	1:B:741:ILE:N	2.74	0.60
2:A:366:SER:OG	2:A:367:GLY:HA3	2.02	0.59
2:A:129:GLN:OE1	2:A:130:TYR:N	2.24	0.59
2:A:195:ILE:HD11	2:A:204:ILE:HG21	1.84	0.58
2:A:362:SER:OG	2:A:366:SER:O	2.12	0.58
2:A:395:LYS:HG2	2:A:399:HIS:ND1	2.17	0.58
2:A:298:ARG:HG2	2:A:302:ASP:OD1	2.03	0.58
2:A:347:LEU:O	6:A:616:HOH:O	2.16	0.58
2:A:389:PHE:HA	2:A:406:CYS:HB3	1.86	0.57
2:A:106:PRO:O	2:A:109:PHE:HB2	2.04	0.57
2:A:333:THR:HG22	2:A:335:ARG:H	1.70	0.57
1:B:827:PRO:HD2	1:B:912:SER:HB3	1.87	0.57
2:A:253:PHE:HB3	2:A:276:TYR:CZ	2.40	0.57
1:B:890:LEU:HD22	1:B:896:TYR:HE2	1.71	0.56
2:A:51:ARG:NH1	6:A:644:HOH:O	2.37	0.56
1:B:860:LEU:HD11	1:B:879:ASP:HB3	1.88	0.56
2:A:129:GLN:HA	2:A:256:LEU:HD13	1.89	0.54
1:B:783:ILE:HG22	1:B:786:LEU:HD21	1.89	0.54
1:B:891:LYS:O	1:B:894:THR:OG1	2.21	0.54
2:A:369:VAL:N	6:A:653:HOH:O	2.40	0.53
1:B:910:THR:OG1	1:B:911:TRP:N	2.40	0.53
1:B:862:THR:HB	1:B:901:MET:HG2	1.90	0.53
2:A:109:PHE:CD2	2:A:120:THR:HB	2.44	0.52
2:A:74:LYS:HB2	2:A:75:PRO:HD2	1.91	0.52
2:A:378:ALA:HB3	2:A:384:TYR:CE1	2.44	0.52
2:A:317:CYS:O	2:A:329:TRP:NE1	2.42	0.52
2:A:417:THR:O	2:A:426:PRO:HD3	2.11	0.51
2:A:291:GLY:HA3	2:A:332:ALA:HB3	1.92	0.50
2:A:107:PRO:O	2:A:110:LEU:HB2	2.11	0.50
2:A:84:GLU:CD	2:A:213:ARG:HH22	2.15	0.50
2:A:352:CYS:O	2:A:353:ARG:NE	2.45	0.49
2:A:431:VAL:HG22	2:A:453:CYS:SG	2.51	0.49
2:A:350:ARG:HH21	2:A:374:ARG:HH21	1.58	0.49
2:A:296:CYS:HB3	2:A:304:LEU:HD23	1.92	0.49
1:B:735:ARG:HD2	1:B:906:ARG:NH2	2.27	0.49
2:A:157:ARG:HD2	2:A:218:GLY:HA3	1.95	0.49
2:A:74:LYS:HB2	2:A:75:PRO:CD	2.42	0.49
2:A:431:VAL:HG12	2:A:432:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:ARG:NH1	1:B:875:TYR:OH	2.46	0.49
1:B:864:ARG:HD3	1:B:911:TRP:CZ2	2.49	0.48
2:A:55:PRO:O	2:A:286:ARG:NH2	2.46	0.48
2:A:127:TYR:HB3	2:A:271:ARG:HD3	1.95	0.48
2:A:153:PHE:O	2:A:217:GLY:N	2.46	0.48
2:A:177:GLN:HG3	2:A:178:PHE:N	2.28	0.48
2:A:212:VAL:O	2:A:215:LEU:HD23	2.14	0.48
2:A:286:ARG:HH21	2:A:286:ARG:HG2	1.79	0.47
2:A:330:GLN:HB2	2:A:338:ASN:HB2	1.96	0.47
2:A:313:ALA:HB3	2:A:319:ARG:HG3	1.96	0.47
2:A:154:CYS:SG	2:A:279:SER:HB3	2.54	0.47
1:B:821:SER:O	1:B:823:PRO:HD3	2.15	0.47
2:A:186:MET:HE2	2:A:255:ARG:HB2	1.97	0.47
1:B:736:PRO:HA	1:B:741:ILE:HG12	1.97	0.47
2:A:177:GLN:HG2	2:A:179:TYR:CZ	2.50	0.47
2:A:94:HIS:ND1	4:A:504:SO4:O4	2.46	0.47
2:A:195:ILE:HG23	2:A:199:ASN:O	2.16	0.47
2:A:412:GLY:HA3	2:A:436:CYS:O	2.15	0.47
2:A:84:GLU:OE1	2:A:213:ARG:NH2	2.48	0.46
1:B:810:GLU:HG3	1:B:811:SER:H	1.79	0.46
2:A:142:LYS:HE3	2:A:287:CYS:SG	2.55	0.46
2:A:350:ARG:HH21	2:A:374:ARG:NH2	2.13	0.46
1:B:740:CYS:HB2	1:B:784:GLU:OE1	2.15	0.46
2:A:127:TYR:CD1	2:A:271:ARG:HB3	2.51	0.46
2:A:157:ARG:HG2	2:A:220:ILE:HD11	1.98	0.46
2:A:395:LYS:HB3	2:A:399:HIS:HB3	1.97	0.45
2:A:158:PRO:HB3	2:A:276:TYR:CE1	2.44	0.45
2:A:296:CYS:HB3	2:A:304:LEU:CD2	2.47	0.45
1:B:890:LEU:HD22	1:B:896:TYR:CE2	2.52	0.45
2:A:177:GLN:HG3	2:A:178:PHE:H	1.82	0.44
2:A:350:ARG:HD3	2:A:374:ARG:NH2	2.32	0.44
2:A:253:PHE:HB3	2:A:276:TYR:CE1	2.53	0.44
2:A:197:LYS:NZ	6:A:650:HOH:O	2.33	0.44
2:A:153:PHE:CE2	2:A:158:PRO:HD3	2.53	0.44
2:A:350:ARG:NH2	2:A:374:ARG:HE	2.16	0.44
2:A:310:HIS:O	2:A:339:GLU:HB2	2.18	0.44
1:B:893:ASN:O	1:B:893:ASN:ND2	2.42	0.43
1:B:730:SER:HB2	1:B:746:THR:OG1	2.18	0.43
2:A:209:HIS:ND1	4:A:505:SO4:O1	2.49	0.43
2:A:128:VAL:O	2:A:132:HIS:HB2	2.19	0.43
2:A:358:LEU:O	2:A:362:SER:OG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:ARG:HA	1:B:736:PRO:HD2	1.93	0.42
1:B:865:TRP:HA	1:B:897:GLU:O	2.19	0.42
2:A:50:PRO:HB3	2:A:310:HIS:CD2	2.55	0.42
2:A:339:GLU:N	2:A:339:GLU:OE1	2.40	0.42
2:A:409:HIS:HA	2:A:410:PRO:HD2	1.81	0.41
2:A:346:ASN:ND2	6:A:641:HOH:O	2.16	0.41
2:A:371:LEU:HD12	2:A:371:LEU:HA	1.71	0.41
2:A:434:ILE:HD13	2:A:434:ILE:HA	1.82	0.41
2:A:447:ARG:O	2:A:449:PRO:HD3	2.21	0.41
2:A:324:HIS:CD2	2:A:342:ALA:HB2	2.56	0.41
2:A:326:ASP:OD1	2:A:367:GLY:HA3	2.21	0.40
2:A:298:ARG:NH2	2:A:304:LEU:HD12	2.36	0.40
2:A:370:CYS:SG	2:A:381:HIS:HA	2.60	0.40
2:A:79:TYR:CZ	2:A:94:HIS:HB2	2.56	0.40
2:A:328:PRO:HG3	2:A:354:PHE:CZ	2.56	0.40
2:A:58:VAL:HG12	2:A:59:ASN:N	2.36	0.40
2:A:184:ARG:HD3	2:A:184:ARG:HH11	1.75	0.40
2:A:389:PHE:CA	2:A:406:CYS:HB3	2.51	0.40
1:B:864:ARG:HD2	1:B:875:TYR:CD1	2.55	0.40
1:B:895:MET:HA	1:B:918:THR:HA	2.02	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	B	186/206 (90%)	184 (99%)	2 (1%)	0	100	100
2	A	408/432 (94%)	388 (95%)	20 (5%)	0	100	100
All	All	594/638 (93%)	572 (96%)	22 (4%)	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	B	169/181 (93%)	147 (87%)	22 (13%)	5	15
2	A	361/378 (96%)	304 (84%)	57 (16%)	3	9
All	All	530/559 (95%)	451 (85%)	79 (15%)	4	11

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	740	CYS
1	B	753	ILE
1	B	771	THR
1	B	775	ASP
1	B	776	SER
1	B	808	LEU
1	B	814	THR
1	B	817	ILE
1	B	824	MET
1	B	825	LEU
1	B	828	VAL
1	B	838	GLU
1	B	841	ARG
1	B	846	ASP
1	B	859	ARG
1	B	866	ARG
1	B	882	SER
1	B	886	THR
1	B	888	THR
1	B	893	ASN
1	B	906	ARG
1	B	921	GLU
2	A	47	HIS
2	A	65	GLU
2	A	66	VAL
2	A	67	LYS
2	A	74	LYS

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Mol	Chain	Res	Type
2	A	83	THR
2	A	90	VAL
2	A	110	LEU
2	A	113	LEU
2	A	121	CYS
2	A	125	ASP
2	A	138	LEU
2	A	146	VAL
2	A	150	SER
2	A	157	ARG
2	A	159	GLU
2	A	176	PHE
2	A	180	SER
2	A	181	THR
2	A	182	GLN
2	A	186	MET
2	A	204	ILE
2	A	210	THR
2	A	219	LEU
2	A	223	SER
2	A	225	LEU
2	A	233	ASP
2	A	240	LEU
2	A	255	ARG
2	A	258	THR
2	A	259	PHE
2	A	266	ASP
2	A	267	SER
2	A	268	GLU
2	A	298	ARG
2	A	300	ARG
2	A	304	LEU
2	A	312	THR
2	A	318	ASP
2	A	343	CYS
2	A	353	ARG
2	A	358	LEU
2	A	361	LEU
2	A	362	SER
2	A	371	LEU
2	A	374	ARG
2	A	377	THR

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Mol	Chain	Res	Type
2	A	390	TYR
2	A	392	ASP
2	A	398	SER
2	A	403	CYS
2	A	406	CYS
2	A	407	ASP
2	A	417	THR
2	A	422	THR
2	A	446	SER
2	A	456	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	916	HIS
2	A	182	GLN
2	A	330	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
3	NAG	A	501	2	14,14,15	0.48	0	15,19,21	0.52	0
3	NAG	A	502	2	14,14,15	1.23	2 (14%)	15,19,21	2.53	5 (33%)
3	NAG	A	503	2	14,14,15	0.78	1 (7%)	15,19,21	0.73	0
4	SO4	A	504	-	4,4,4	0.17	0	6,6,6	0.27	0
4	SO4	A	505	-	4,4,4	0.12	0	6,6,6	0.30	0
4	SO4	A	506	-	4,4,4	0.09	0	6,6,6	0.38	0
4	SO4	A	507	-	4,4,4	0.13	0	6,6,6	0.20	0
4	SO4	A	508	-	4,4,4	0.15	0	6,6,6	0.20	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	A	501	2	-	0/6/23/26	0/1/1/1
3	NAG	A	502	2	-	0/6/23/26	0/1/1/1
3	NAG	A	503	2	-	0/6/23/26	0/1/1/1
4	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0
4	SO4	A	506	-	-	0/0/0/0	0/0/0/0
4	SO4	A	507	-	-	0/0/0/0	0/0/0/0
4	SO4	A	508	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAG	C2-N2	-2.78	1.41	1.46
3	A	503	NAG	O5-C1	2.36	1.47	1.43
3	A	502	NAG	C1-C2	2.74	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C2-N2-C7	-5.62	115.82	123.04
3	A	502	NAG	O3-C3-C2	-2.19	104.78	109.11
3	A	502	NAG	O5-C5-C6	3.94	115.87	107.35
3	A	502	NAG	C4-C3-C2	4.08	117.58	111.23
3	A	502	NAG	C1-O5-C5	4.22	117.60	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	SO4	1	0
4	A	505	SO4	1	0
4	A	507	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	192/206 (93%)	0.28	2 (1%) 84 82	14, 54, 88, 103	0
2	A	412/432 (95%)	0.18	7 (1%) 73 70	9, 30, 72, 90	0
All	All	604/638 (94%)	0.21	9 (1%) 76 74	9, 37, 79, 103	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	823	PRO	3.8
2	A	414	ALA	3.2
2	A	364	ARG	2.7
2	A	421	THR	2.6
1	B	880	THR	2.5
2	A	397	ILE	2.3
2	A	415	GLY	2.2
2	A	387	GLU	2.0
2	A	81	VAL	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 carbohydrates 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	502	14/15	0.54	0.49	3.78	32,47,62,70	0
5	CA	A	509	1/1	0.96	0.25	1.06	15,15,15,15	0
3	NAG	A	503	14/15	0.78	0.23	0.28	46,58,68,73	0
4	SO4	A	506	5/5	0.98	0.22	0.14	16,16,21,26	0
4	SO4	A	505	5/5	0.96	0.13	-3.08	34,35,45,49	0
4	SO4	A	504	5/5	0.93	0.14	-	52,60,60,68	0
4	SO4	A	507	5/5	0.92	0.13	-	66,70,78,80	0
3	NAG	A	501	14/15	0.95	0.23	-	38,40,46,50	0
4	SO4	A	508	5/5	0.91	0.16	-	70,80,89,91	0

## 6.5 Other polymers

There are no such residues in this entry.