



# Full wwPDB X-ray Structure Validation Report i

Sep 4, 2014 – 04:47 PM EDT

PDB ID : 4URT  
Title : The crystal structure of a fragment of netrin-1 in complex with FN5- FN6 of DCC  
Authors : Finci, L.I.; Krueger, N.; Sun, X.; Zhang, J.; Chegkazi, M.; Wu, Y.; Schenk, G.; Mertens, H.D.T.; Svergun, D.I.; Zhang, Y.; Wang, J.-h.; Meijers, R.  
Deposited on : 2014-07-02  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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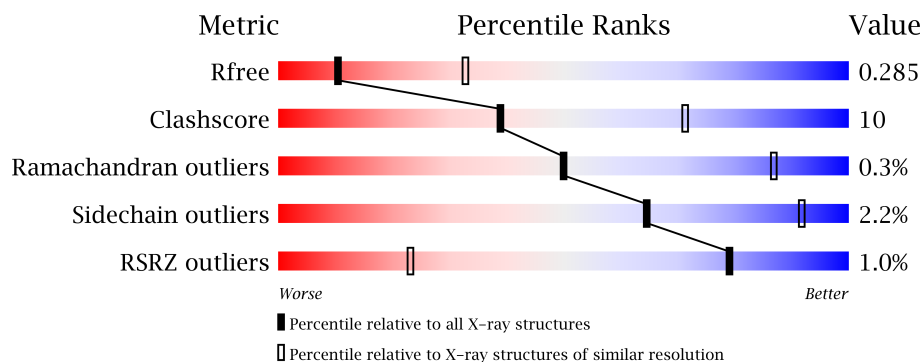
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	420	
2	B	206	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CL	A	1466	-	X
6	SO4	A	1468	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5129 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			Total	C	N	O	S			
1	A	420	3318	2026	637	615	40	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	GLU	-	EXPRESSION TAG	UNP O95631
A	455	LEU	-	EXPRESSION TAG	UNP O95631
A	456	HIS	-	EXPRESSION TAG	UNP O95631
A	457	HIS	-	EXPRESSION TAG	UNP O95631
A	458	HIS	-	EXPRESSION TAG	UNP O95631

- Molecule 2 is a protein called NETRIN RECEPTOR DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	206	1634	1042	278	307	7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1045	LEU	-	EXPRESSION TAG	UNP P43146
B	1046	GLU	-	EXPRESSION TAG	UNP P43146
B	1047	VAL	-	EXPRESSION TAG	UNP P43146
B	1048	LEU	-	EXPRESSION TAG	UNP P43146
B	1049	PHE	-	EXPRESSION TAG	UNP P43146
B	1050	ALA	-	EXPRESSION TAG	UNP P43146

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

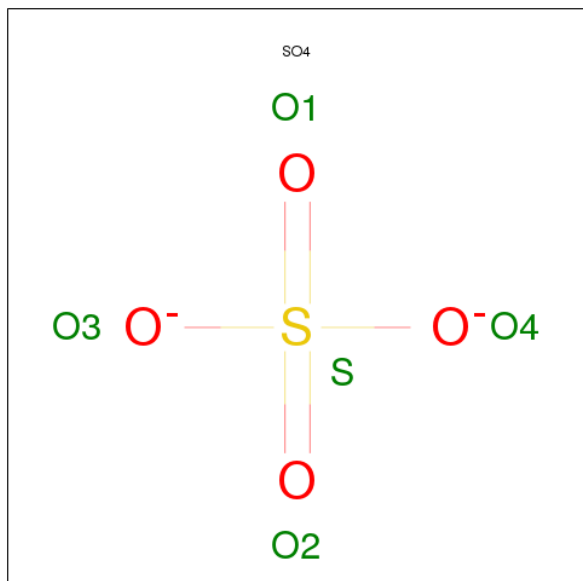
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



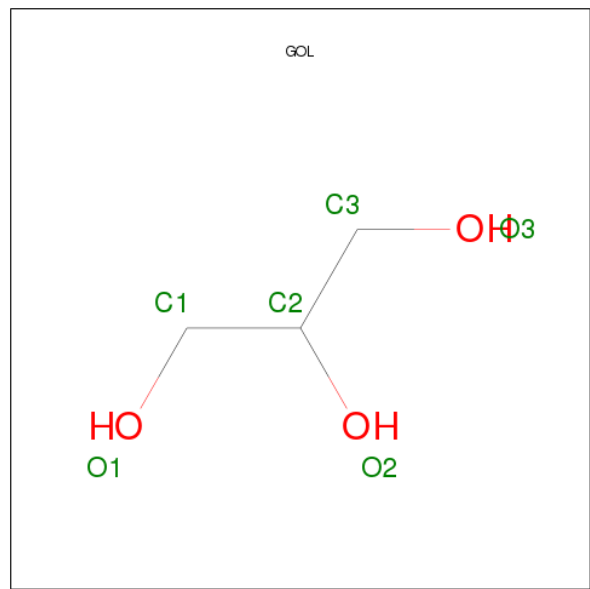
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



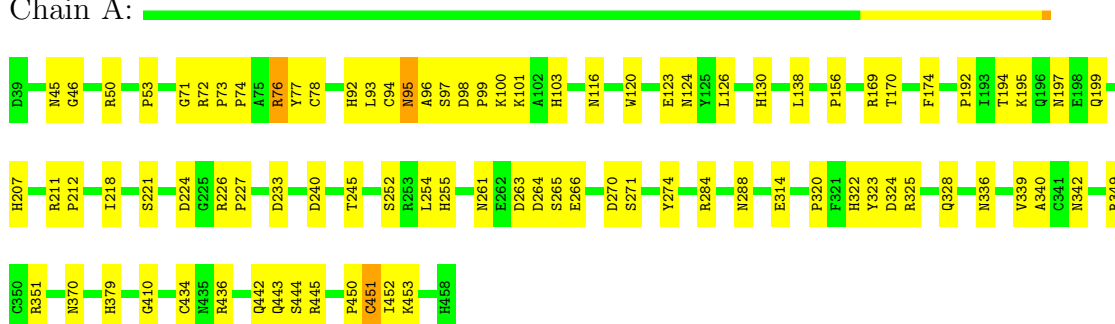
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

### 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.

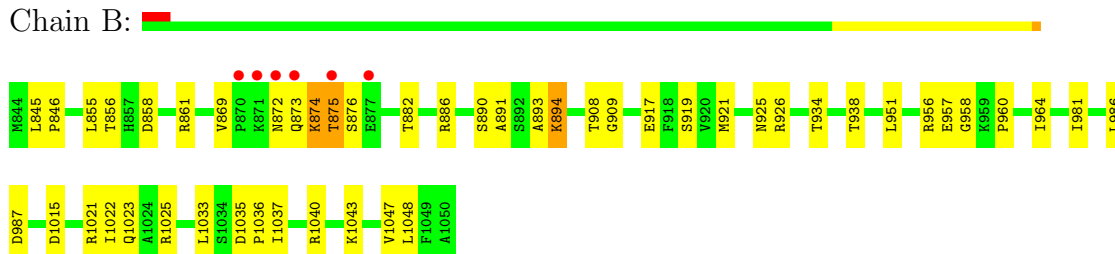
#### • Molecule 1: NETRIN-1

Chain A:



#### • Molecule 2: NETRIN RECEPTOR DCC

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.65Å 87.41Å 155.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.66 – 3.10 77.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (77.66-3.10) 99.2 (77.66-3.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.230 , 0.265 0.243 , 0.285	Depositor DCC
$R_{free}$ test set	1099 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.5	EDS
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 21391 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, CL, SO4, 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	0.22	0/3402	0.39	0/4602
2	B	0.21	0/1673	0.41	0/2280
All	All	0.22	0/5075	0.40	0/6882

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3318	0	3113	62	0
2	B	1634	0	1644	31	0
3	A	84	0	75	15	0
4	A	1	0	0	0	0
5	A	1	0	0	4	0
6	A	80	0	0	2	0
6	B	5	0	0	0	0
7	B	6	0	8	1	0
All	All	5129	0	4840	97	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (97) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:ASN:HD21	3:A:1461:NAG:C1	1.29	1.46
1:A:116:ASN:ND2	3:A:1461:NAG:C1	1.86	1.37
1:A:116:ASN:HD21	3:A:1461:NAG:C2	1.74	1.01
1:A:323:TYR:OH	5:A:1466:CL:CL	2.40	0.74
1:A:116:ASN:HD22	3:A:1461:NAG:C1	1.95	0.74
1:A:221:SER:HB3	1:A:224:ASP:HB2	1.68	0.74
1:A:450:PRO:O	1:A:452:ILE:N	2.19	0.71
3:A:1462:NAG:C1	3:A:1462:NAG:H83	2.21	0.71
1:A:324:ASP:HB3	1:A:339:VAL:HG23	1.73	0.70
1:A:288:ASN:ND2	1:A:314:GLU:O	2.27	0.68
1:A:342:ASN:HB3	1:A:379:HIS:HD2	1.62	0.65
2:B:938:THR:H	7:B:2052:GOL:H2	1.62	0.64
2:B:845:LEU:HD12	2:B:846:PRO:HD2	1.81	0.63
2:B:886:ARG:NE	2:B:917:GLU:OE1	2.34	0.60
2:B:874:LYS:HG3	2:B:875:THR:HG22	1.83	0.60
1:A:443:GLN:HA	1:A:451:CYS:HA	1.84	0.59
3:A:1461:NAG:C3	3:A:1461:NAG:H83	2.34	0.58
3:A:1461:NAG:H83	3:A:1461:NAG:O3	2.05	0.56
1:A:53:PRO:O	1:A:284:ARG:NH1	2.38	0.56
1:A:116:ASN:HD21	3:A:1461:NAG:C3	2.17	0.56
2:B:1021:ARG:HD3	2:B:1036:PRO:HG3	1.88	0.56
1:A:78:CYS:N	1:A:270:ASP:O	2.36	0.55
1:A:322:HIS:HA	1:A:340:ALA:HA	1.88	0.55
1:A:443:GLN:HA	1:A:451:CYS:H	1.72	0.54
1:A:76:ARG:NH2	1:A:266:GLU:O	2.41	0.54
3:A:1462:NAG:C1	3:A:1462:NAG:C8	2.86	0.54
1:A:320:PRO:HD3	5:A:1466:CL:CL	2.46	0.53
1:A:192:PRO:O	1:A:197:ASN:ND2	2.41	0.52
1:A:194:THR:OG1	1:A:195:LYS:N	2.42	0.52
1:A:156:PRO:HB3	1:A:274:TYR:HE1	1.73	0.52
2:B:886:ARG:HB2	2:B:893:ALA:HB1	1.92	0.52
2:B:1023:GLN:HB3	2:B:1033:LEU:HD23	1.93	0.51
1:A:320:PRO:CD	5:A:1466:CL:CL	2.97	0.50
1:A:78:CYS:HB2	1:A:271:SER:HB3	1.93	0.50
2:B:960:PRO:HB3	2:B:1048:LEU:HD21	1.93	0.49
1:A:199:GLN:NE2	1:A:240:ASP:OD2	2.45	0.49
2:B:1021:ARG:HH11	2:B:1036:PRO:HD3	1.78	0.49
1:A:95:ASN:OD1	1:A:98:ASP:N	2.46	0.48
1:A:74:PRO:HG3	1:A:95:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:ASP:O	1:A:265:SER:N	2.47	0.48
1:A:450:PRO:O	1:A:452:ILE:HG23	2.14	0.48
1:A:349:ARG:NH1	2:B:909:GLY:O	2.41	0.48
1:A:103:HIS:HB3	1:A:120:TRP:HA	1.96	0.47
2:B:872:ASN:HB3	2:B:873:GLN:HG3	1.96	0.47
1:A:45:ASN:N	1:A:46:GLY:HA2	2.30	0.46
1:A:207:HIS:HB3	1:A:218:ILE:HD13	1.97	0.46
1:A:325:ARG:HG2	1:A:339:VAL:HG22	1.98	0.46
2:B:1015:ASP:OD1	2:B:1040:ARG:NH1	2.41	0.46
2:B:894:LYS:HE2	2:B:894:LYS:O	2.16	0.45
1:A:123:GLU:HA	1:A:124:ASN:HA	1.61	0.45
1:A:98:ASP:HA	1:A:99:PRO:HD3	1.83	0.45
1:A:126:LEU:HD12	1:A:130:HIS:HB3	1.98	0.45
2:B:919:SER:HB3	2:B:934:THR:HG22	1.99	0.45
1:A:92:HIS:HE1	1:A:101:LYS:HE2	1.83	0.44
2:B:890:SER:OG	2:B:891:ALA:N	2.44	0.44
2:B:925:ASN:HA	2:B:926:ARG:HA	1.56	0.44
1:A:74:PRO:HG2	3:A:1459:NAG:H82	1.99	0.44
1:A:444:SER:OG	1:A:445:ARG:N	2.51	0.44
1:A:443:GLN:HA	1:A:451:CYS:N	2.31	0.44
1:A:436:ARG:NH1	6:A:1478:SO4:O2	2.44	0.44
1:A:71:GLY:HA3	1:A:96:ALA:HB2	1.98	0.44
5:A:1466:CL:CL	2:B:858:ASP:OD1	2.72	0.44
1:A:100:LYS:HD3	1:A:100:LYS:HA	1.86	0.43
1:A:211:ARG:HB2	1:A:212:PRO:HD3	1.99	0.43
2:B:875:THR:HG23	2:B:876:SER:H	1.82	0.43
1:A:444:SER:HB2	1:A:453:LYS:HG3	2.00	0.43
2:B:951:LEU:HD22	2:B:1022:ILE:HG22	1.99	0.43
1:A:138:LEU:HB2	1:A:245:THR:O	2.19	0.43
1:A:77:TYR:CE1	1:A:94:CYS:HB2	2.54	0.43
1:A:169:ARG:HG3	1:A:170:THR:HG23	2.01	0.43
1:A:252:SER:O	1:A:274:TYR:OH	2.34	0.43
1:A:370:ASN:ND2	6:A:1471:SO4:O4	2.52	0.43
2:B:882:THR:HB	2:B:921:MET:HG2	2.00	0.43
2:B:1043:LYS:HB2	2:B:1047:VAL:HG23	2.00	0.43
1:A:328:GLN:HG3	1:A:336:ASN:HB3	2.00	0.42
3:A:1461:NAG:H83	3:A:1461:NAG:H3	2.00	0.42
1:A:95:ASN:OD1	1:A:95:ASN:C	2.57	0.42
1:A:95:ASN:OD1	1:A:97:SER:N	2.52	0.42
2:B:1035:ASP:N	2:B:1035:ASP:OD1	2.51	0.42
1:A:50:ARG:NH1	1:A:233:ASP:OD2	2.52	0.42
1:A:72:ARG:HA	1:A:73:PRO:HA	1.89	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:981:ILE:HD11	2:B:1025:ARG:HD2	2.02	0.42
1:A:351:ARG:NH2	2:B:908:THR:O	2.53	0.42
2:B:957:GLU:HA	2:B:958:GLY:HA2	1.57	0.41
3:A:1461:NAG:O4	3:A:1462:NAG:H83	2.20	0.41
1:A:254:LEU:HG	1:A:274:TYR:CZ	2.55	0.41
2:B:872:ASN:CB	2:B:873:GLN:HA	2.50	0.41
1:A:98:ASP:HB2	3:A:1459:NAG:H61	2.01	0.41
2:B:856:THR:OG1	2:B:858:ASP:OD1	2.38	0.41
1:A:116:ASN:ND2	3:A:1461:NAG:H3	2.36	0.41
1:A:226:ARG:HA	1:A:227:PRO:HD2	1.67	0.41
1:A:410:GLY:HA3	1:A:434:CYS:O	2.21	0.41
2:B:855:LEU:HD11	2:B:861:ARG:HB2	2.03	0.41
2:B:956:ARG:HD2	2:B:964:ILE:HD11	2.02	0.40
2:B:951:LEU:HB3	2:B:1037:ILE:HD12	2.02	0.40
2:B:987:ASP:N	2:B:987:ASP:OD1	2.55	0.40
1:A:116:ASN:ND2	3:A:1461:NAG:C5	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/420 (100%)	377 (90%)	40 (10%)	2 (0%)	38	81
2	B	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
All	All	623/626 (100%)	559 (90%)	62 (10%)	2 (0%)	50	87

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	CYS
1	A	264	ASP

### 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	365/364 (100%)	358 (98%)	7 (2%)	69	92
2	B	182/182 (100%)	177 (97%)	5 (3%)	57	89
All	All	547/546 (100%)	535 (98%)	12 (2%)	64	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ARG
1	A	93	LEU
1	A	95	ASN
1	A	174	PHE
1	A	255	HIS
1	A	261	ASN
1	A	442	GLN
2	B	869	VAL
2	B	874	LYS
2	B	875	THR
2	B	894	LYS
2	B	986	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	189	HIS
1	A	239	GLN
1	A	261	ASN
1	A	379	HIS
1	A	442	GLN
1	A	456	HIS
2	B	857	HIS
2	B	1023	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

6 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	1459	1,3	12,14,15	0.37	0	15,19,21	0.76	0
3	NAG	A	1460	3	12,14,15	0.33	0	15,19,21	0.28	0
3	NAG	A	1461	3	12,14,15	0.75	0	15,19,21	0.96	0
3	NAG	A	1462	3	12,14,15	0.62	0	15,19,21	1.22	2 (13%)
3	NAG	A	1463	1,3	12,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	A	1464	3	12,14,15	0.36	0	15,19,21	0.30	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	1459	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1460	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1461	3	-	1/6/23/26	0/1/1/1
3	NAG	A	1462	3	-	2/6/23/26	0/1/1/1
3	NAG	A	1463	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1464	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1462	NAG	O5-C5-C4	-3.09	106.73	110.65
3	A	1462	NAG	O5-C5-C6	3.02	110.15	106.98
3	A	1463	NAG	O5-C5-C4	-3.01	106.84	110.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1462	NAG	C8-C7-N2-C2
3	A	1462	NAG	O7-C7-N2-C2
3	A	1461	NAG	O7-C7-N2-C2

There are no ring outliers.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
6	SO4	A	1467	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	1468	-	4,4,4	0.22	0	6,6,6	0.09	0
6	SO4	A	1469	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	1470	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	1471	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	A	1472	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	1473	-	4,4,4	0.23	0	6,6,6	0.07	0
6	SO4	A	1474	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	1475	-	4,4,4	0.20	0	6,6,6	0.07	0
6	SO4	A	1476	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	1477	-	4,4,4	0.22	0	6,6,6	0.07	0
6	SO4	A	1478	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	1479	-	4,4,4	0.22	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	A	1480	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	1481	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	A	1483	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	B	2051	-	4,4,4	0.24	0	6,6,6	0.10	0
7	GOL	B	2052	-	5,5,5	0.34	0	5,5,5	0.25	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
6	SO4	A	1467	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1468	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1469	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1470	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1471	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1472	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1473	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1474	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1475	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1476	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1477	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1478	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1479	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1480	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1481	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1483	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2051	-	-	0/0/0/0	0/0/0/0
7	GOL	B	2052	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	420/420 (100%)	-0.03	0 100 100	42, 79, 139, 172	0
2	B	206/206 (100%)	0.22	6 (2%) 49 7	48, 79, 131, 182	0
All	All	626/626 (100%)	0.05	6 (0%) 79 23	42, 79, 139, 182	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	870	PRO	4.6
2	B	872	ASN	4.1
2	B	871	LYS	3.9
2	B	873	GLN	3.7
2	B	877	GLU	2.2
2	B	875	THR	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	1461	14/15	0.27	-0.08	134,160,164,174	0
3	NAG	A	1459	14/15	0.21	-0.41	129,137,149,156	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1463	14/15	0.16	-1.26	109,119,132,134	0
3	NAG	A	1462	14/15	0.22	-	150,161,175,175	0
3	NAG	A	1460	14/15	0.31	-	118,137,142,147	0
3	NAG	A	1464	14/15	0.16	-	114,129,138,139	0

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	A	1466	1/1	0.41	3.12	95,95,95,95	0
6	SO4	A	1468	5/5	0.28	2.54	88,98,112,150	0
7	GOL	B	2052	6/6	0.29	0.96	75,75,75,82	0
6	SO4	A	1480	5/5	0.20	0.93	116,116,131,158	0
6	SO4	A	1475	5/5	0.26	0.59	103,105,122,163	0
6	SO4	A	1481	5/5	0.16	-0.52	68,77,84,106	0
6	SO4	A	1471	5/5	0.17	-0.66	70,70,70,91	0
4	CA	A	1465	1/1	0.14	-0.76	103,103,103,103	0
6	SO4	A	1479	5/5	0.17	-0.94	100,115,129,131	0
6	SO4	A	1474	5/5	0.22	-0.96	108,109,130,143	0
6	SO4	A	1472	5/5	0.17	-0.97	87,97,98,101	0
6	SO4	A	1478	5/5	0.12	-1.31	89,94,97,114	0
6	SO4	A	1476	5/5	0.16	-1.39	80,85,108,118	0
6	SO4	A	1467	5/5	0.15	-1.56	83,89,119,125	0
6	SO4	A	1477	5/5	0.15	-1.73	81,94,138,142	0
6	SO4	A	1473	5/5	0.17	-1.78	77,77,77,82	0
6	SO4	A	1469	5/5	0.14	-1.92	87,89,108,113	0
6	SO4	A	1483	5/5	0.14	-2.13	107,121,129,173	0
6	SO4	A	1470	5/5	0.14	-2.30	92,92,102,105	0
6	SO4	B	2051	5/5	0.15	-2.48	78,78,89,119	0

## 6.5 Other polymers

There are no such residues in this entry.