



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZYJ  
Title : NETRING1 IN COMPLEX WITH NGL1  
Authors : Seiradake, E.; Coles, C.H.; Perestenko, P.V.; Harlos, K.; Mcilhinney, R.A.J.; Aricescu, A.R.; Jones, E.Y.  
Deposited on : 2011-08-23  
Resolution : 3.25 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

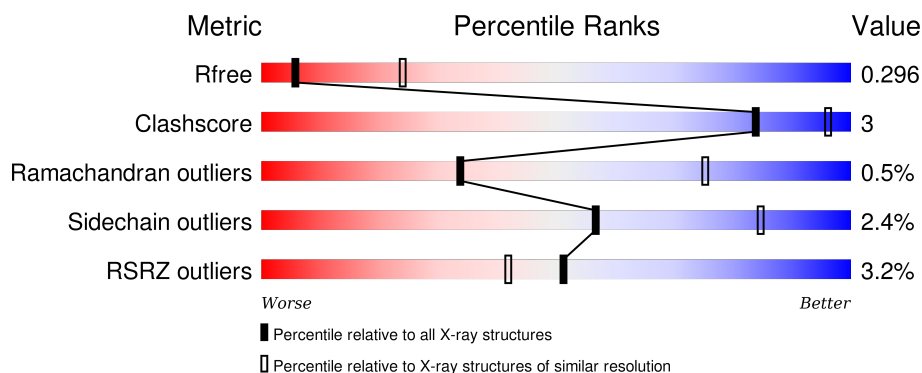
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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. 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	440	<div> <div>3%</div> <div>80% 10% 10%</div> </div>
1	C	440	<div> <div>4%</div> <div>82% 8% 10%</div> </div>
2	B	426	<div> <div>3%</div> <div>69% 8% 23%</div> </div>
2	D	426	<div> <div>%</div> <div>66% 10% 23%</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	B	1370	-	-	-	X
3	NAG	B	1371	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11388 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 LEUCINE-RICH REPEAT-CONTAINING PROTEIN 4C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3063	1938	539	566	20			
1	C	396	Total	C	N	O	S	0	0	0
			3061	1935	540	566	20			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	EXPRESSION TAG	UNP Q9HCJ2
A	14	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
A	15	ILE	-	EXPRESSION TAG	UNP Q9HCJ2
A	16	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	17	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
A	18	SER	-	EXPRESSION TAG	UNP Q9HCJ2
A	19	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
A	20	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
A	21	MET	-	EXPRESSION TAG	UNP Q9HCJ2
A	22	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
A	23	ALA	-	EXPRESSION TAG	UNP Q9HCJ2
A	24	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	25	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	26	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	27	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
A	28	SER	-	EXPRESSION TAG	UNP Q9HCJ2
A	29	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	30	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	31	SER	-	EXPRESSION TAG	UNP Q9HCJ2
A	32	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
A	33	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	34	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
A	35	MET	-	EXPRESSION TAG	UNP Q9HCJ2
A	36	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
A	37	CYS	-	EXPRESSION TAG	UNP Q9HCJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	38	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
A	39	ALA	-	EXPRESSION TAG	UNP Q9HCJ2
A	40	GLU	-	EXPRESSION TAG	UNP Q9HCJ2
A	41	THR	-	EXPRESSION TAG	UNP Q9HCJ2
A	42	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
A	43	SER	-	EXPRESSION TAG	UNP Q9HCJ2
A	445	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
A	446	THR	-	EXPRESSION TAG	UNP Q9HCJ2
A	447	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
A	448	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
A	449	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
A	450	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
A	451	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
A	452	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	13	MET	-	EXPRESSION TAG	UNP Q9HCJ2
C	14	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
C	15	ILE	-	EXPRESSION TAG	UNP Q9HCJ2
C	16	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	17	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
C	18	SER	-	EXPRESSION TAG	UNP Q9HCJ2
C	19	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
C	20	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
C	21	MET	-	EXPRESSION TAG	UNP Q9HCJ2
C	22	PRO	-	EXPRESSION TAG	UNP Q9HCJ2
C	23	ALA	-	EXPRESSION TAG	UNP Q9HCJ2
C	24	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	25	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	26	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	27	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
C	28	SER	-	EXPRESSION TAG	UNP Q9HCJ2
C	29	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	30	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	31	SER	-	EXPRESSION TAG	UNP Q9HCJ2
C	32	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
C	33	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	34	LEU	-	EXPRESSION TAG	UNP Q9HCJ2
C	35	MET	-	EXPRESSION TAG	UNP Q9HCJ2
C	36	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
C	37	CYS	-	EXPRESSION TAG	UNP Q9HCJ2
C	38	VAL	-	EXPRESSION TAG	UNP Q9HCJ2
C	39	ALA	-	EXPRESSION TAG	UNP Q9HCJ2
C	40	GLU	-	EXPRESSION TAG	UNP Q9HCJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	THR	-	EXPRESSION TAG	UNP Q9HCJ2
C	42	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
C	43	SER	-	EXPRESSION TAG	UNP Q9HCJ2
C	445	GLY	-	EXPRESSION TAG	UNP Q9HCJ2
C	446	THR	-	EXPRESSION TAG	UNP Q9HCJ2
C	447	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	448	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	449	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	450	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	451	HIS	-	EXPRESSION TAG	UNP Q9HCJ2
C	452	HIS	-	EXPRESSION TAG	UNP Q9HCJ2

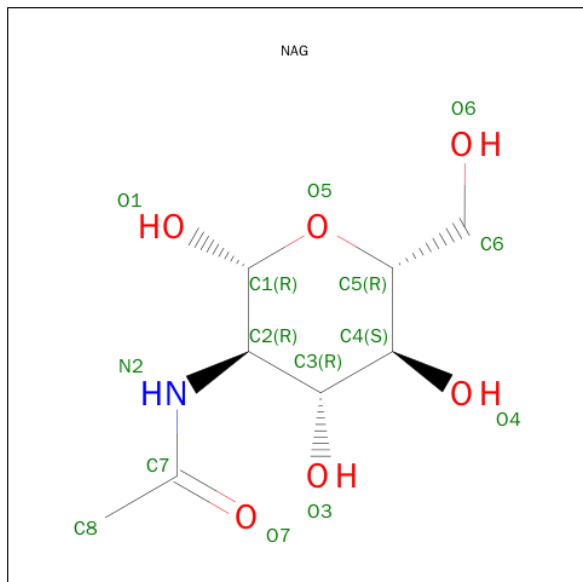
- Molecule 2 is a protein called NETRIN-G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	326	Total	C	N	O	S	0	0	0
			2567	1630	421	492	24			
2	D	326	Total	C	N	O	S	0	0	0
			2561	1627	418	492	24			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	430	THR	-	EXPRESSION TAG	UNP Q9Y2I2
B	431	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	432	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	433	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	434	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	435	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	436	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
B	360	ALA	THR	ENGINEERED MUTATION	UNP Q9Y2I2
B	363	ALA	THR	ENGINEERED MUTATION	UNP Q9Y2I2
D	430	THR	-	EXPRESSION TAG	UNP Q9Y2I2
D	431	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	432	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	433	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	434	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	435	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	436	HIS	-	EXPRESSION TAG	UNP Q9Y2I2
D	360	ALA	THR	ENGINEERED MUTATION	UNP Q9Y2I2
D	363	ALA	THR	ENGINEERED MUTATION	UNP Q9Y2I2

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

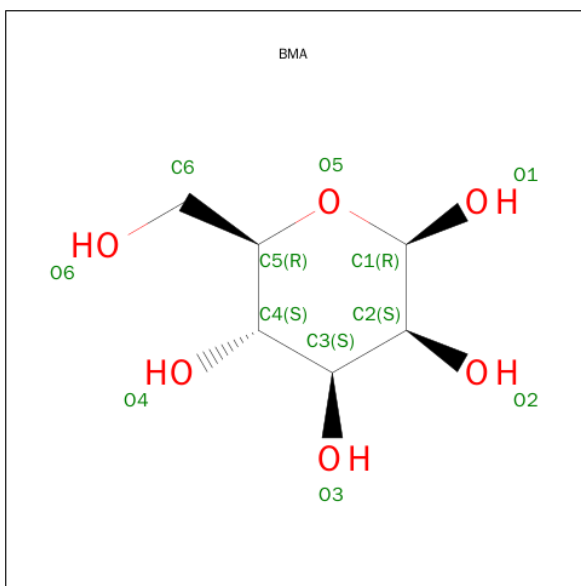


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

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

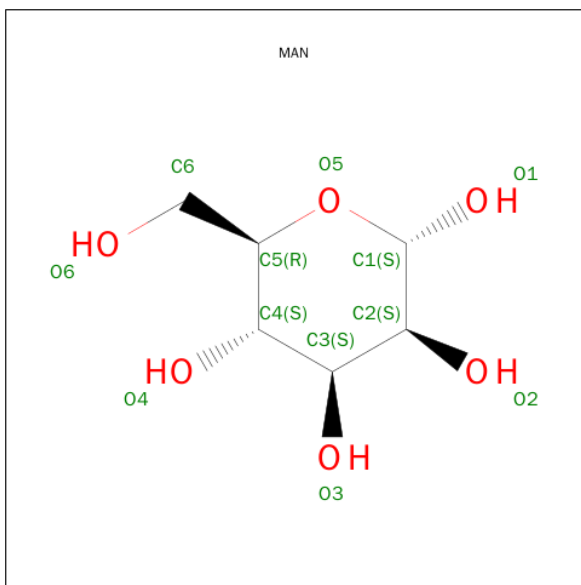
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



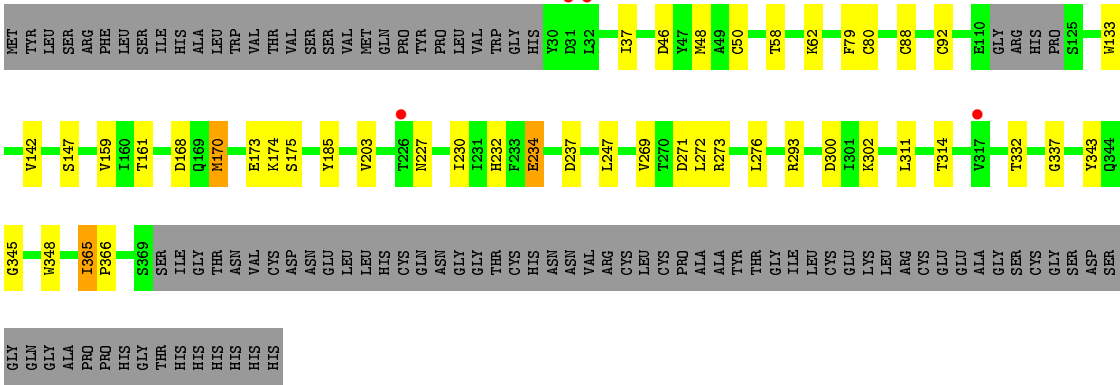
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			11	6	5		





HIS  
HIS

• Molecule 2: NETRIN-G1



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.42Å 204.43Å 288.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 3.25 29.44 – 3.25	Depositor EDS
% Data completeness (in resolution range)	91.3 (29.44-3.25) 91.3 (29.44-3.25)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.24Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.256 , 0.268 0.283 , 0.296	Depositor DCC
$R_{free}$ test set	1961 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	4 of 39036 reflections (0.010%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.92 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4288e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, BMA, NAG, MAN

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	0.37	0/3129	0.56	0/4276
1	C	0.37	0/3126	0.56	0/4271
2	B	0.36	0/2636	0.56	0/3591
2	D	0.37	0/2630	0.58	0/3584
All	All	0.37	0/11521	0.56	0/15722

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3063	0	3007	21	0
1	C	3061	0	3011	15	0
2	B	2567	0	2428	13	0
2	D	2561	0	2416	17	0
3	A	14	0	13	0	0
3	B	42	0	39	1	0
3	C	14	0	13	0	0
3	D	42	0	39	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	D	11	0	10	1	0
6	D	11	0	10	0	0
All	All	11388	0	10986	68	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 3.

All (68) 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:D:37:ILE:HG12	2:D:46:ASP:HB2	1.81	0.63
1:C:223:GLU:HG2	1:C:247:LYS:HB2	1.80	0.63
2:D:161:THR:HG22	2:D:230:ILE:HG12	1.81	0.62
1:A:45:GLN:N	1:A:75:SER:HG	1.98	0.62
2:B:175:SER:HB3	2:B:271:ASP:HB2	1.83	0.61
2:B:161:THR:HG22	2:B:230:ILE:HG12	1.82	0.59
1:A:256:GLN:HG3	1:A:278:ASN:HD22	1.69	0.58
1:A:223:GLU:HG2	1:A:247:LYS:HB2	1.86	0.57
1:A:374:LYS:HA	1:A:410:THR:HG22	1.87	0.56
2:B:142:VAL:HB	2:B:276:LEU:HD12	1.87	0.56
2:D:170:MET:HG3	2:D:276:LEU:HD23	1.87	0.56
2:D:174:LYS:HG3	2:D:269:VAL:HG12	1.88	0.56
2:D:175:SER:HB3	2:D:271:ASP:HB2	1.89	0.55
1:A:145:VAL:HG13	1:A:170:ARG:HE	1.73	0.54
2:D:50:CYS:HB3	2:D:314:THR:HG23	1.90	0.54
1:C:176:ARG:HG2	1:C:201:TYR:HB3	1.89	0.54
2:D:234:GLU:HB3	2:D:237:ASP:HB2	1.90	0.52
1:C:163:ILE:HD12	1:C:188:ILE:HG12	1.90	0.52
2:D:343:TYR:HA	2:D:366:PRO:HA	1.91	0.51
1:A:198:ASN:HA	1:A:220:LYS:HD3	1.92	0.51
2:B:255:GLY:HA2	2:B:354:LEU:HD11	1.93	0.51
1:C:234:ILE:HD12	1:C:258:ILE:HG12	1.93	0.51
2:B:50:CYS:HB3	2:B:314:THR:HG23	1.94	0.50
2:D:173:GLU:HB2	2:D:273:ARG:HB3	1.94	0.50
2:B:169:GLN:HB3	2:B:277:LEU:HB2	1.93	0.50
3:B:1370:NAG:H4	3:B:1372:NAG:C1	2.42	0.50
1:A:82:ASN:HA	1:A:106:GLN:HB2	1.93	0.50
1:C:281:LEU:HD13	1:C:381:LEU:HD21	1.94	0.49
2:B:234:GLU:HB3	2:B:237:ASP:HB2	1.95	0.49
1:A:234:ILE:HD12	1:A:258:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG23	1:A:84:HIS:HB3	1.94	0.48
1:C:145:VAL:HG13	1:C:170:ARG:HE	1.79	0.48
1:A:273:ASN:HA	1:A:297:HIS:HB2	1.96	0.47
2:D:345:GLY:HA3	2:D:365:ILE:HG22	1.96	0.47
2:D:142:VAL:HB	2:D:276:LEU:HD12	1.98	0.46
2:D:159:VAL:HB	2:D:302:LYS:HB2	1.97	0.46
2:B:159:VAL:HB	2:B:302:LYS:HB2	1.97	0.46
1:A:106:GLN:HA	1:A:130:GLU:HB2	1.96	0.46
2:D:80:CYS:HB2	2:D:293:ARG:HA	1.97	0.46
2:D:62:LYS:HG3	2:D:147:SER:HB2	1.98	0.46
3:D:1372:NAG:H4	5:D:1373:BMA:C1	2.47	0.45
1:C:106:GLN:HA	1:C:130:GLU:HB2	1.99	0.44
2:B:84:ASN:HB2	2:B:87:MET:HB2	2.00	0.44
1:A:281:LEU:HD13	1:A:381:LEU:HD21	1.99	0.44
2:D:203:VAL:HG21	2:D:234:GLU:HB2	1.99	0.44
1:C:421:THR:HG22	1:C:443:VAL:H	1.82	0.44
2:B:343:TYR:HA	2:B:366:PRO:HA	1.99	0.44
1:A:297:HIS:HA	1:A:326:CYS:HB3	2.00	0.44
2:B:173:GLU:HB2	2:B:273:ARG:HB3	1.99	0.43
1:C:236:PRO:HA	1:C:262:ALA:HA	2.00	0.43
1:C:152:GLU:HG2	1:C:176:ARG:HB2	2.00	0.43
1:A:386:TRP:CD2	1:A:411:LEU:HD12	2.54	0.42
2:D:79:PHE:CE2	2:D:92:CYS:HB2	2.55	0.42
1:C:272:ILE:HG23	1:C:296:ILE:HG23	2.01	0.42
2:B:62:LYS:HG3	2:B:147:SER:HB2	2.00	0.42
1:C:374:LYS:HA	1:C:410:THR:HG22	2.02	0.42
1:A:163:ILE:HD12	1:A:188:ILE:HG12	2.00	0.41
2:B:170:MET:HG3	2:B:276:LEU:HD23	2.02	0.41
1:A:331:ASN:HA	1:A:337:LYS:HG3	2.03	0.41
1:A:123:LEU:HB3	1:A:126:LEU:HB2	2.03	0.41
1:C:198:ASN:HA	1:C:220:LYS:HD3	2.03	0.41
2:D:337:GLY:HA2	2:D:348:TRP:CZ2	2.56	0.41
1:A:152:GLU:HG2	1:A:176:ARG:HB2	2.03	0.41
1:C:331:ASN:HA	1:C:337:LYS:HG3	2.02	0.41
1:C:212:ILE:HD13	1:C:238:SER:HB3	2.03	0.40
1:A:93:VAL:HG13	1:A:118:GLY:HA3	2.04	0.40
1:A:130:GLU:HG2	1:A:154:TRP:HD1	1.86	0.40
1:A:236:PRO:HA	1:A:262:ALA:HA	2.03	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	392/440 (89%)	366 (93%)	24 (6%)	2 (0%)	34	75
1	C	392/440 (89%)	371 (95%)	19 (5%)	2 (0%)	34	75
2	B	322/426 (76%)	302 (94%)	20 (6%)	0	100	100
2	D	322/426 (76%)	299 (93%)	20 (6%)	3 (1%)	21	64
All	All	1428/1732 (82%)	1338 (94%)	83 (6%)	7 (0%)	34	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	227	ASN
2	D	234	GLU
1	A	402	ARG
1	C	321	PRO
1	C	402	ARG
1	A	321	PRO
2	D	58	THR

### 5.3.2 Protein sidechains [i](#)

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	341/393 (87%)	336 (98%)	5 (2%)	72	90
1	C	341/393 (87%)	337 (99%)	4 (1%)	78	92
2	B	281/378 (74%)	273 (97%)	8 (3%)	51	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	280/378 (74%)	267 (95%)	13 (5%)	33	72
All	All	1243/1542 (81%)	1213 (98%)	30 (2%)	57	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	CYS
1	A	171	ILE
1	A	315	TRP
1	A	330	CYS
1	A	381	LEU
2	B	32	LEU
2	B	37	ILE
2	B	44	VAL
2	B	88	CYS
2	B	133	TRP
2	B	176	LEU
2	B	185	TYR
2	B	232	HIS
1	C	62	CYS
1	C	171	ILE
1	C	282	LEU
1	C	423	MET
2	D	48	MET
2	D	88	CYS
2	D	133	TRP
2	D	168	ASP
2	D	170	MET
2	D	185	TYR
2	D	232	HIS
2	D	247	LEU
2	D	272	LEU
2	D	300	ASP
2	D	311	LEU
2	D	332	THR
2	D	365	ILE

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	278	ASN

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Mol	Chain	Res	Type
2	B	101	HIS
2	B	227	ASN
2	B	330	ASN
1	C	252	GLN
1	C	278	ASN
2	D	51	GLN
2	D	101	HIS
2	D	330	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	1445	-	14,14,15	0.41	0	15,19,21	1.23	1 (6%)
3	NAG	B	1370	-	14,14,15	0.42	0	15,19,21	1.22	1 (6%)
3	NAG	B	1371	-	14,14,15	0.42	0	15,19,21	1.21	1 (6%)
3	NAG	B	1372	-	14,14,15	0.41	0	15,19,21	1.23	1 (6%)
3	NAG	C	1445	-	14,14,15	0.41	0	15,19,21	1.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	1370	-	14,14,15	0.40	0	15,19,21	1.22	1 (6%)
3	NAG	D	1371	-	14,14,15	0.44	0	15,19,21	1.19	1 (6%)
3	NAG	D	1372	-	14,14,15	0.42	0	15,19,21	1.16	1 (6%)
5	BMA	D	1373	-	11,11,12	0.38	0	14,15,17	1.07	0
6	MAN	D	1374	-	11,11,12	0.41	0	14,15,17	1.02	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	1445	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1370	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1371	-	-	0/6/23/26	0/1/1/1
3	NAG	B	1372	-	-	0/6/23/26	0/1/1/1
3	NAG	C	1445	-	-	0/6/23/26	0/1/1/1
3	NAG	D	1370	-	-	0/6/23/26	0/1/1/1
3	NAG	D	1371	-	-	0/6/23/26	0/1/1/1
3	NAG	D	1372	-	-	0/6/23/26	0/1/1/1
5	BMA	D	1373	-	-	0/2/19/22	0/1/1/1
6	MAN	D	1374	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1370	NAG	C4-C3-C2	-2.44	107.44	111.23
3	A	1445	NAG	C4-C3-C2	-2.43	107.46	111.23
3	B	1372	NAG	C4-C3-C2	-2.43	107.46	111.23
3	D	1370	NAG	C4-C3-C2	-2.40	107.49	111.23
3	B	1371	NAG	C4-C3-C2	-2.37	107.54	111.23
3	D	1371	NAG	C4-C3-C2	-2.37	107.55	111.23
3	C	1445	NAG	C4-C3-C2	-2.34	107.58	111.23
3	D	1372	NAG	C4-C3-C2	-2.23	107.77	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1370	NAG	1	0
3	B	1372	NAG	1	0
3	D	1372	NAG	1	0
5	D	1373	BMA	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 ⓘ

### 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	396/440 (90%)	0.15	15 (3%) 44 34	80, 107, 141, 179	0
1	C	396/440 (90%)	0.13	16 (4%) 42 32	68, 98, 154, 203	0
2	B	326/426 (76%)	0.18	11 (3%) 49 39	76, 100, 125, 146	0
2	D	326/426 (76%)	0.04	4 (1%) 81 72	61, 89, 116, 141	0
All	All	1444/1732 (83%)	0.13	46 (3%) 51 42	61, 98, 142, 203	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	THR	5.6
1	A	366	THR	5.2
1	C	444	THR	4.7
1	A	369	MET	4.1
1	C	324	THR	4.1
1	C	352	TYR	4.0
1	C	367	GLU	3.8
1	A	370	ALA	3.8
2	D	226	THR	3.5
1	C	369	MET	3.5
1	C	322	SER	3.4
1	A	325	ALA	3.3
1	A	371	ALA	3.3
1	C	427	MET	3.2
1	A	427	MET	3.2
1	C	371	ALA	3.0
1	C	350	THR	3.0
1	A	318	ASP	2.9
1	A	324	THR	2.7
2	B	228	SER	2.6
2	B	227	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	444	THR	2.6
2	B	317	VAL	2.6
2	B	31	ASP	2.5
2	B	223	GLY	2.4
2	D	317	VAL	2.4
1	A	436	THR	2.4
1	C	348	TYR	2.4
2	B	45	TRP	2.3
2	B	32	LEU	2.3
1	C	418	VAL	2.3
1	C	353	ALA	2.2
1	A	437	ALA	2.2
1	A	322	SER	2.2
1	C	280	THR	2.2
2	B	245	PRO	2.2
2	D	32	LEU	2.1
2	B	286	VAL	2.1
2	B	226	THR	2.1
1	A	392	THR	2.1
1	A	416	VAL	2.1
1	A	326	CYS	2.0
2	B	36	GLN	2.0
2	D	31	ASP	2.0
1	C	443	VAL	2.0
1	C	327	CYS	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 ⓘ

There are no carbohydrates in this entry.

## 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	1371	14/15	0.68	0.49	2.44	138,138,139,139	0
3	NAG	B	1370	14/15	0.71	0.32	2.10	133,134,134,134	0
3	NAG	D	1371	14/15	0.69	0.37	1.68	122,123,124,124	0
3	NAG	D	1370	14/15	0.79	0.29	1.60	124,124,125,125	0
4	CA	B	1373	1/1	0.95	0.08	-3.24	102,102,102,102	0
4	CA	D	1375	1/1	0.94	0.07	-3.50	88,88,88,88	0
3	NAG	B	1372	14/15	0.68	0.26	-	123,124,124,124	0
3	NAG	C	1445	14/15	0.71	0.55	-	144,144,144,145	0
3	NAG	D	1372	14/15	0.75	0.38	-	116,117,118,118	0
3	NAG	A	1445	14/15	0.64	0.42	-	132,133,133,133	0
5	BMA	D	1373	11/12	0.83	0.30	-	107,108,108,108	0
6	MAN	D	1374	11/12	0.68	0.41	-	139,139,139,139	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.