



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 3ZYI / pdb_00003zyi
Title : NetrinG2 in complex with NGL2
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 : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

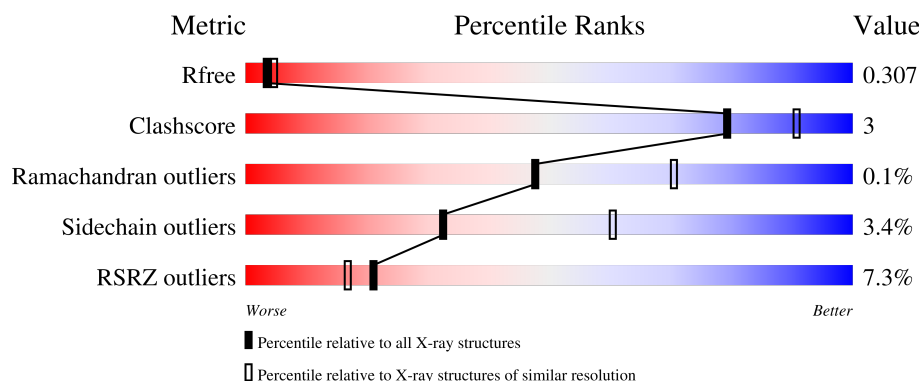
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	452	6% 78% 8% 13%
2	B	353	7% 80% 6% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5450 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3066	1945	530	565	26	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9HBW1
A	446	THR	-	expression tag	UNP Q9HBW1
A	447	HIS	-	expression tag	UNP Q9HBW1
A	448	HIS	-	expression tag	UNP Q9HBW1
A	449	HIS	-	expression tag	UNP Q9HBW1
A	450	HIS	-	expression tag	UNP Q9HBW1
A	451	HIS	-	expression tag	UNP Q9HBW1
A	452	HIS	-	expression tag	UNP Q9HBW1

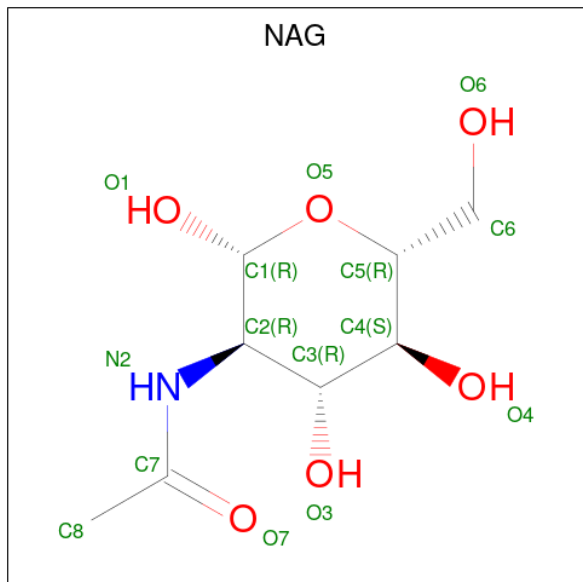
- Molecule 2 is a protein called NETRIN-G2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	303	2345	1472	406	442	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

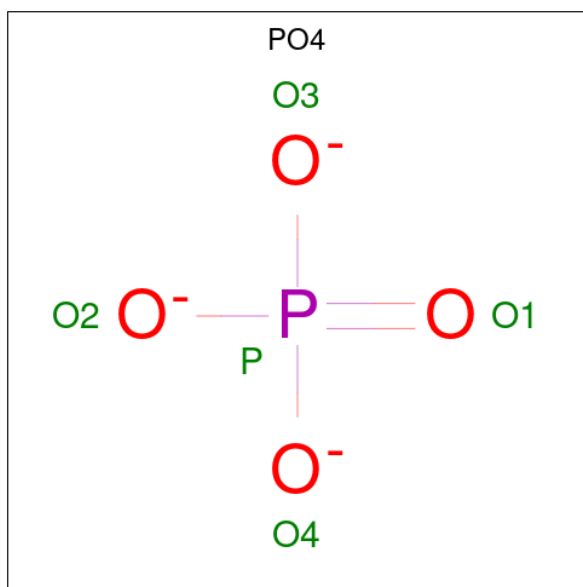
Chain	Residue	Modelled	Actual	Comment	Reference
B	346	GLY	-	expression tag	UNP Q96CW9
B	347	THR	-	expression tag	UNP Q96CW9
B	348	HIS	-	expression tag	UNP Q96CW9
B	349	HIS	-	expression tag	UNP Q96CW9
B	350	HIS	-	expression tag	UNP Q96CW9
B	351	HIS	-	expression tag	UNP Q96CW9
B	352	HIS	-	expression tag	UNP Q96CW9
B	353	HIS	-	expression tag	UNP Q96CW9

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	75.42Å 153.39Å 158.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.95 – 2.60 28.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.95-2.60) 98.6 (28.95-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.243 , 0.287 0.258 , 0.307	Depositor DCC
R_{free} test set	1439 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5450	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, PO4, CA

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	0.72	0/3141	1.20	6/4279 (0.1%)
2	B	0.69	0/2404	1.12	2/3264 (0.1%)
All	All	0.71	0/5545	1.16	8/7543 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	GLN	N-CA-C	6.30	118.23	111.36
2	B	210	HIS	N-CA-C	6.30	119.73	109.59
1	A	326	CYS	N-CA-C	5.98	121.49	113.72
1	A	211	MET	N-CA-C	5.62	116.49	109.57
2	B	250	THR	N-CA-C	-5.46	107.17	113.88
1	A	217	LEU	CA-C-N	5.36	128.09	120.53
1	A	217	LEU	C-N-CA	5.36	128.09	120.53
1	A	116	VAL	N-CA-C	5.26	115.89	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3066	0	2952	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2345	0	2132	8	1
3	A	14	0	13	0	0
3	B	14	0	13	1	0
4	A	10	0	0	0	1
5	B	1	0	0	0	0
All	All	5450	0	5110	28	1

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 (28) 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:A:55:GLN:HB2	1:A:57:SER:OG	1.68	0.93
1:A:55:GLN:O	1:A:56:PHE:HB2	1.75	0.85
1:A:304:CYS:HA	1:A:308:ILE:HG12	1.60	0.84
1:A:83:MET:HE1	2:B:78:SER:HB2	1.64	0.80
2:B:56:PRO:HD3	3:B:1348:NAG:H81	1.72	0.70
1:A:55:GLN:CB	1:A:57:SER:OG	2.40	0.69
1:A:55:GLN:O	1:A:56:PHE:CB	2.50	0.58
1:A:83:MET:HE3	1:A:105:GLN:HB3	1.91	0.52
1:A:205:MET:HE1	2:B:72:GLU:HG2	1.90	0.52
1:A:222:GLU:HG3	1:A:246:LYS:HB3	1.94	0.50
1:A:175:ARG:HG2	1:A:200:TYR:HB3	1.93	0.49
1:A:162:ILE:HD12	1:A:187:ILE:HG12	1.93	0.49
1:A:304:CYS:HA	1:A:308:ILE:CG1	2.37	0.48
2:B:51:LYS:HB2	2:B:126:SER:HB2	1.96	0.47
1:A:89:MET:HG3	1:A:113:GLN:HB3	1.97	0.47
2:B:120:GLU:HG2	2:B:257:LEU:HA	1.96	0.46
2:B:321:LYS:HA	2:B:324:ARG:CZ	2.46	0.45
2:B:53:LYS:HB2	2:B:124:THR:HB	1.99	0.45
1:A:90:ILE:HG22	1:A:118:ALA:HB1	1.99	0.43
1:A:81:ASN:HA	1:A:105:GLN:HB2	2.02	0.42
1:A:280:SER:HB3	1:A:379:MET:HE2	2.02	0.41
1:A:162:ILE:HG22	1:A:191:ALA:HB1	2.01	0.41
1:A:259:ARG:HH22	1:A:376:THR:HG22	1.85	0.41
2:B:41:PRO:HG2	2:B:287:CYS:HB2	2.03	0.41
1:A:246:LYS:HG3	1:A:270:GLU:HB3	2.02	0.41
1:A:192:PHE:HB3	1:A:217:LEU:HD21	2.03	0.40
1:A:151:GLU:HG2	1:A:175:ARG:HB2	2.03	0.40
1:A:398:HIS:HB3	1:A:401:ILE:O	2.20	0.40

All (1) 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:B:321:LYS:O	4:A:1444:PO4:O2[8_555]	1.72	0.48

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	391/452 (86%)	367 (94%)	24 (6%)	0	100	100
2	B	295/353 (84%)	282 (96%)	12 (4%)	1 (0%)	36	58
All	All	686/805 (85%)	649 (95%)	36 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	46	LEU

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	340/399 (85%)	327 (96%)	13 (4%)	29	56
2	B	242/311 (78%)	235 (97%)	7 (3%)	37	65
All	All	582/710 (82%)	562 (97%)	20 (3%)	32	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	55	GLN
1	A	56	PHE
1	A	57	SER
1	A	79	TYR
1	A	112	ARG
1	A	242	SER
1	A	249	VAL
1	A	296	HIS
1	A	362	LEU
1	A	364	ILE
1	A	376	THR
1	A	416	LEU
2	B	21	ILE
2	B	49	TYR
2	B	164	TYR
2	B	173	GLU
2	B	194	LEU
2	B	315	ASP
2	B	321	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	168	ASN
1	A	253	GLN
1	A	413	HIS
2	B	128	ASN
2	B	210	HIS
2	B	267	GLN
2	B	270	ASN
2	B	304	GLN
2	B	310	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1348	2	14,14,15	0.51	0	17,19,21	1.11	2 (11%)
3	NAG	A	1442	1	14,14,15	0.45	0	17,19,21	1.13	2 (11%)
4	PO4	A	1444	-	4,4,4	2.04	1 (25%)	6,6,6	0.90	0
4	PO4	A	1443	-	4,4,4	1.96	1 (25%)	6,6,6	0.47	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	1348	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1442	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1443	PO4	P-O1	3.52	1.58	1.50
4	A	1444	PO4	P-O1	3.38	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1348	NAG	C4-C3-C2	-2.18	107.82	111.02
3	A	1442	NAG	C8-C7-N2	2.18	119.73	116.12
3	A	1442	NAG	C4-C3-C2	-2.14	107.88	111.02
3	B	1348	NAG	C6-C5-C4	-2.02	108.06	113.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1442	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1348	NAG	1	0
4	A	1444	PO4	0	1

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/452 (87%)	0.63	27 (6%) 23 19	38, 54, 76, 98	0
2	B	303/353 (85%)	0.84	24 (7%) 18 14	43, 61, 86, 110	0
All	All	698/805 (86%)	0.72	51 (7%) 21 17	38, 57, 80, 110	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	TRP	7.5
1	A	319	ILE	4.3
1	A	441	VAL	4.2
2	B	102	GLY	4.0
2	B	62	GLY	3.9
2	B	237	LEU	3.7
1	A	340	LEU	3.6
2	B	18	ASP	3.4
2	B	347	THR	3.4
2	B	321	LYS	3.3
2	B	221	ILE	3.3
1	A	97	HIS	3.2
2	B	238	GLU	3.1
1	A	180	GLU	2.9
2	B	185	MET	2.9
2	B	187	SER	2.9
2	B	318	LYS	2.8
1	A	98	LEU	2.8
2	B	143	TYR	2.8
2	B	183	ARG	2.8
1	A	44	GLN	2.7
1	A	316	ARG	2.6
1	A	161	SER	2.6
2	B	19	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	329	ARG	2.6
1	A	419	THR	2.6
2	B	125	LEU	2.6
1	A	56	PHE	2.6
2	B	101	GLU	2.5
1	A	365	SER	2.5
2	B	241	LYS	2.5
2	B	182	ALA	2.4
1	A	369	MET	2.4
1	A	65	GLY	2.4
2	B	192	ARG	2.3
1	A	170	VAL	2.3
1	A	121	GLY	2.3
1	A	370	ALA	2.2
2	B	40	GLN	2.2
1	A	53	SER	2.2
1	A	64	ARG	2.2
1	A	95	PHE	2.2
2	B	21	ILE	2.2
2	B	343	ALA	2.2
1	A	71	GLN	2.2
1	A	318	TYR	2.1
1	A	72	GLY	2.1
1	A	100	HIS	2.1
1	A	145	TYR	2.1
1	A	417	SER	2.0
1	A	315	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	1442	14/15	0.75	0.16	88,89,91,92	0
3	NAG	B	1348	14/15	0.75	0.19	76,79,82,83	0
4	PO4	A	1444	5/5	0.76	0.18	66,72,72,73	0
4	PO4	A	1443	5/5	0.90	0.11	63,69,70,70	0
5	CA	B	1349	1/1	0.97	0.04	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.